201-16174B

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IUCLID

Data Set

Existing Chemical	:	ID: 298-07-7
CAS No.	:	298-07-7
EINECS Name	:	bis(2-ethylhexyl) hydrogen phosphate
EC No.	:	206-056-4
TSCA Name	:	Phosphoric acid, bis(2-ethylhexyl) ester
Molecular Formula	:	C16H35O4P

Producer related part

Company	:	Rhodia UK limited
Creation date	:	02.12.2005

Substance related part

Company	:	Rhodia UK limited
Creation date	:	02.12.2005
Status	:	
Memo	:	
Printing date	:	14.12.2005
Revision date	:	
Date of last update	:	14.12.2005
Number of pages	:	51
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	manufacturer
Name	:	Rhodia Inc.
Contact person	:	Ian BARTLETT
Date	:	
Street	:	8 Cedar Brook Drive
Town	:	08512 Cranbury, NJ
Country	:	United States
Phone	:	609-860-3913
Telefax	:	609-860-0076
Telex	:	
Cedex	:	
Email	:	ian.bartlett@us.rhodia.com
Homepage	:	

06.12.2005

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name	:	bis(2-ethylhexyl) hydrogen phosphate
Smiles Code	:	O=P(OCC(CCCC)CC)(OCC(CCCC)CC)O
Molecular formula	:	C16 H35 O4 P1
Molecular weight	:	322.43
Petrol class	:	

05.12.2005

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	typical for marketed substance
Substance type	:	organic
Physical status	:	liquid
Purity	:	95 - 98 % w/w
Colour	:	Colourless to pale yellow
Odour	:	Slight

08.12.2005

Purity type	:	
Substance type	:	inorganic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Source : Bayer AG Leverkusen
Bayer Corporation Pittsburgh

06.12.2005

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1-HEXANOL, 2-ETHYL-, HYDROGEN PHOSPHATE

06.12.2005

BIS(2-ETHYLHEXYL) HYDROGEN PHOSPHATE

03.08.1992

BIS(2-ETHYLHEXYL) PHOSPHATE

03.08.1992

BIS(2-ETHYLHEXYL) PHOSPHORIC ACID

03.08.1992

DEHPA

06.12.2005

DI(2-ETHYLHEXYL) PHOSPHORIC ACID

03.08.1992

DI-2-ETHYLHEXYL HYDROGEN PHOSPHATE

03.08.1992

DIOCTYLPHOSPHAT

03.08.1992

PHOSPHORIC ACID BIS(ETHYLHEXYL) ESTER

03.08.1992

PHOSPHORIC ACID, BIS(2-ETHYLHEXYL) ESTER

14.12.2005

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	1070-03-7
EC-No	:	213-967-0
EINECS-Name	:	2-ethylhexyl dihydrogen phosphate
Molecular formula	:	C8 H19 O4 P
Value	:	= 1 - 3 % w/w

08.12.2005

Purity	:	typical for marketed substance
CAS-No	:	78-42-2
EC-No	:	201-116-6
EINECS-Name	:	tris(2-ethylhexyl) phosphate
Molecular formula	:	C24 H51 O4 P
Value	:	= .4 - 2.5 % w/w

08.12.2005

Purity	:	typical for marketed substance
CAS-No	:	123-04-6
EC-No	:	204-594-4
EINECS-Name	:	3-(chloromethyl)heptane
Molecular formula	:	C8 H17 Cl
Value	:	= .2 - 1 % w/w

08.12.2005

Purity	:	typical for marketed substance
CAS-No	:	104-76-7
EC-No	:	203-234-3
EINECS-Name	:	2-ethylhexan-1-ol
Molecular formula	:	C8 H18 O
Value	:	< .5 % w/w

14.12.2005

Purity	:	typical for marketed substance
CAS-No	:	10143-60-9
EC-No	:	233-412-6
EINECS-Name	:	bis(2-ethylhexyl) ether
Molecular formula	:	C16 H34 O
Value	:	< .5 % w/w

14.12.2005

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark	:	Human exposure is limited to accidental contact during drum filling or handling. Inhalative exposure can be excluded as the vapour pressure is very low.
Source	:	Bayer AG Leverkusen Bayer Corporation Pittsburgh

21.07.1997

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

Type of search	:	Internal and External
Chapters covered	:	3, 4, 5
Date of search	:	13.09.2005

06.12.2005

Type of search	:	Internal and External
Chapters covered	:	2
Date of search	:	13.09.2005

06.12.2005

1.13 REVIEWS

2.1 MELTING POINT

Value : = -50 °C

Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Data from industry.

Flag : Critical study for SIDS endpoint

06.12.2005 (1) (2)

Value : = -60 °C

Reliability : (2) valid with restrictions
Cited in standard data source.

06.12.2005 (3)

Value : = -60 °C

Reliability : (2) valid with restrictions
Cited in standard data source.

06.12.2005 (4) (5)

Value : = -60 °C

Reliability : (2) valid with restrictions
Cited in standard data source.

06.12.2005 (6)

Value : < -60 °C

Reliability : (4) not assignable
Data from industry.

14.12.2005 (7)

Value : 86.3 °C
Sublimation :
Method : other: calculated
Year :
GLP :
Test substance : other TS: molecular structure

Method : Estimated with MPBPWIN programme v1.41, US-EPA/Syracuse Research Corporation.

Result : Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 120.14 deg C (Gold and Ogle Method)
Mean Melt Pt : 97.57 deg C (Joback; Gold,Ogle Methods)
Selected MP: 86.28 deg C (Weighted Value)

Reliability : (2) valid with restrictions
Accepted calculation method

14.12.2005

2.2 BOILING POINT

Decomposition : yes
Method : other
Year :
GLP : no data
Test substance : other TS

Method : Differential thermoanalysis (DTA) at a heating rate of 5 °C/mn in a glass ampule.
Result : Decomposition temperature = 240 °C.
Test substance : Baysolvex D2EHPA Di-(2-ethylhexyl)-phosphat.
Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Data from industry.
Flag : Critical study for SIDS endpoint
14.12.2005 (1) (2)

Decomposition : yes
Method : other: DIN 51758
Year :
GLP :
Test substance :

Result : Decomposes at 240 °C, at 1000 hPa.
Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Data from industry.
14.12.2005 (8) (9)

Value : = 155 °C at .02 hPa

Reliability : (2) valid with restrictions
Cited in standard data source.
13.12.2005 (10)

Value : 400.4 °C at 1013 hPa
Decomposition :
Method : other: calculated
Year :
GLP :
Test substance : other TS: molecular structure

Method : Estimated with MPBPWIN programme v1.41, US-EPA/Syracuse Research Corporation.
Reliability : (2) valid with restrictions
Accepted calculation method
06.12.2005

2.3 DENSITY

Type : relative density
Value : = .96 at 20 °C

Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Data from industry.
14.12.2005 (1) (2)

Type : relative density
Value : = .973 at 25 °C

Reliability : (2) valid with restrictions
Cited in standard data source.
14.12.2005 (3)

Type : relative density
Value : = .974 at 20 °C

Reliability : (4) not assignable

Cited in SDS
14.12.2005 (11)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : < .1 hPa at 20 °C

Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Data from industry.
Flag : Critical study for SIDS endpoint
06.12.2005 (1) (2)

Value : = .00000024 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance : other TS: molecular structure

Method : Estimated with MPBPWIN programme v1.41, US-EPA/Syracuse Research Corporation.
Result : Vapor Pressure Estimations (25 deg C):
(Using BP: 400.41 deg C (estimated))
(MP not used for liquids)
VP: 2.74E-008 mm Hg (Antoine Method)
VP: 1.8E-007 mm Hg (Modified Grain Method)
VP: 1.67E-005 mm Hg (Mackay Method)
Selected VP: 1.8E-007 mm Hg (Modified Grain Method)
Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
14.12.2005

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 2.67 at °C
pH value :
Method : other (measured)
Year :
GLP : no data
Test substance : no data

Reliability : (2) valid with restrictions
Experimental data measured at Chemicals Inspection and Testing Institute, JP.
Flag : Critical study for SIDS endpoint
06.12.2005 (7)

Partition coefficient :
Log pow : 6.07 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP :

Test substance	:	other TS: molecular structure
Method	:	Estimated with KOWWIN programme v1.67, US-EPA/Syracuse Research Corporation.
Reliability	:	(2) valid with restrictions Accepted calculation method

06.12.2005

Partition coefficient	:	
Log pow	:	4.6 - 5.4 at °C
pH value	:	
Method	:	other (calculated): Leo, A.: CLOGP-3.54 MedChem Software 1989. Daylight, Chemical Information Systems, Claremont, CA 91711, USA
Year	:	
GLP	:	
Test substance	:	
Source	:	Bayer AG Leverkusen Bayer Corporation Pittsburgh
Reliability	:	(2) valid with restrictions Accepted calculation method

06.12.2005 (12)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 210 mg/l at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Reliability	:	(2) valid with restrictions Cited in peer reviewed secondary source. Data from industry.
Flag	:	Critical study for SIDS endpoint

14.12.2005 (13) (2)

Solubility in	:	Water
Value	:	= 182 mg/l at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	no data
Reliability	:	(2) valid with restrictions Experimental data measured at Chemicals Inspection and Testing Institute, JP.

14.12.2005 (7)

Solubility in : Water
Value : = .01 other: % w/w at 20 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Reliability : (2) valid with restrictions
Cited in standard data source.

14.12.2005 (4) (5)

Solubility in : Water
Value : < 1 g/l at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Data from industry.

14.12.2005 (9) (14)

Solubility in : Water
Value : = 422.5 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance :

Method : Estimated with WSKOW programme v1.41, US-EPA/Syracuse Research Corporation.
Result : Log Kow used by Water solubility estimates: 2.67 (user entered)

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

Melting Pt (Tm) = -50.00 deg C (Use Tm = 25 for all liquids)

Correction(s): Value
--- ---
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -2.883
Water Solubility at 25 deg C (mg/L): 422.5

Reliability : (2) valid with restrictions
Accepted calculation method

14.12.2005

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	1.47 at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: molecular structure
Method	:	Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2005 ACD/Labs).
Result	:	0.024 g/L at pH 1, 25 deg C 0.077 g/L at pH 2, 25 deg C 0.61 g/L at pH 3, 25 deg C 5.5 g/L at pH 4, 25 deg C 28 g/L at pH 5, 25 deg C 52 g/L at pH 6, 25 deg C 55 g/L at pH 7, 25 deg C 55 g/L at pH 8, 25 deg C 55 g/L at pH 9, 25 deg C 55 g/L at pH 10, 25 deg C 0.45 g/L in unbuffered Water, pH 2.87, 25 deg C
Reliability	:	(2) valid with restrictions Accepted calculation method

14.12.2005

Solubility in	:	Water
Value	:	.05926 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: molecular structure
Method	:	Estimated with WSKOW programme v1.41, US-EPA/Syracuse Research Corporation.
Result	:	Log Kow (estimated) : 6.07 Log Kow (experimental): not available from database Log Kow used by Water solubility estimates: 6.07 Equation Used to Make Water Sol estimate: Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW Log Water Solubility (in moles/L) : -6.736 Water Solubility at 25 deg C (mg/L): 0.05926
Reliability	:	(2) valid with restrictions Accepted calculation method

14.12.2005

2.6.2 SURFACE TENSION

Test type :
Value : = 20 mN/m at 20 °C
Concentration :

Reliability : (2) valid with restrictions
Cited in standard data source.

06.12.2005 (4) (5)

2.7 FLASH POINT

Value : = 198 °C
Type :

Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Data from industry.

07.12.2005 (1) (2)

Value : = 196 °C
Type :

Reliability : (2) valid with restrictions
Cited in standard data source.

07.12.2005 (3)

Value : = 196 °C
Type : open cup

Reliability : (2) valid with restrictions
Cited in standard data source.

07.12.2005 (15) (4)

Value : = 150 °C
Type : closed cup

Reliability : (4) not assignable
Cited in SDS

14.12.2005 (11)

Value : = 191.7 °C
Type :
Method : other: calculated
Year :
GLP :
Test substance : other TS: molecular structure

Method : Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2005 ACD/Labs).
Result : 191.7 +/- 23.2 °C
Reliability : (2) valid with restrictions
Accepted calculation method

14.12.2005

2.8 AUTO FLAMMABILITY

Value : > 300 °C at
Method : other: DIN 51794
Year :
GLP :
Test substance :

Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Data from industry.

14.12.2005 (1) (2)

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant : 3.49
Method : other: measured
Year :
GLP :
Test substance :

Test condition : Measured in 75 % ethanol.
Measured at 25 °C.
Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Primary source not retrieved.

14.12.2005 (2) (16)

Acid-base constant : 1.47 +/- 0.50 at 25 °C
Method : other: calculated
Year :
GLP :
Test substance : other TS: molecular structure

Method : Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2005 ACD/Labs).
Reliability : (2) valid with restrictions
Accepted calculation method

14.12.2005

Remark : At environmentally relevant pH values (pH 5-9) bis(2-ethylhexyl) hydrogen phosphate exists almost entirely (> 99.9 %) in anionic form.
The saturated aqueous solution has a pH of about 3.

14.12.2005 (13) (2)

2.13 VISCOSITY

Value : = 47.32 - mPa s (dynamic) at 21 °C
Result :

Reliability : (2) valid with restrictions

Cited in standard data source.

08.12.2005 (4) (5)

Value : = 56 - mPa s (dynamic) at 20 °C
Result :

Result : 56 mPa.s at 20 °C
160 mPa.s at 0 °C
Reliability : (4) not assignable
Cited in SDS

08.12.2005 (11)

Value : = 124.1 - mPa s (dynamic) at 40 °C
Result :

Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Primary source not retrieved.

14.12.2005 (2) (17)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm^3
Rate constant	:	.0000000000653784 cm^3/(molecule*sec)
Degradation	:	50 % after 3.9 hour(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: molecular structure
Method	:	Estimated with AOPWIN programme v1.91, US-EPA/Syracuse Research Corporation.
Result	:	OVERALL OH Rate Constant = 65.3784 E-12 cm3/molecule-sec HALF-LIFE = 0.164 Days = 3.9 hours (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 0.245 Days = 5.9 hours (24-hr day; 0.5E6 OH/cm3)
Reliability	:	(2) valid with restrictions Accepted calculation method
Flag	:	Critical study for SIDS endpoint

14.12.2005

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	other: air - water - soil - sediment
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: calculated
Year	:	

Method : Estimated with EPIWINWIN programme v3.12, US-EPA/Syracuse Research Corporation.

Result :

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.302	3.93	1000
Water	24.5	360	1000
Soil	75	720	1000
Sediment	0.226	3.24e+003	0

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.94	3.93	1000
Water	5.19	360	0
Soil	91.8	720	0
Sediment	0.0479	3.24e+003	0

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000188	3.93	0
Water	99.1	360	1000
Soil	0.00587	720	0
Sediment	0.916	3.24e+003	0

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00207	3.93	0
Water	1.72	360	0
Soil	98.3	720	1000
Sediment	0.0159	3.24e+003	0

Test condition : INPUTS:

Chem Name : Phosphoric acid, bis(2-ethylhexyl) ester
Molecular Wt: 322.43
Henry's LC : 4.11e-008 atm-m3/mole (Henrywin program)
Vapor Press : 1.8e-007 mm Hg (Mpbpwin program)
Log Kow : 2.67 (user-entered)
Soil Koc : 192 (calc by model from Log Kow)

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 3.926
Water: 360
Soil: 720
Sediment: 3240
Biowin 3 estimate: 3.083 (approx. amount of time needed for degradation: weeks)

Reliability : (2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint
12.12.2005

3.3.2 DISTRIBUTION

Media : water - air
Method : other (calculation)
Year :

Method : Calculated from:
VP = 2.4 E-07 hPa (estimated with MPBPWIN v1.41)
WS = 210 mg/l (experimental value)

Result : Henry's Law constant (HLC) =
3.636 E-010 atm.m3/mol
3.683 E-05 Pa.m3/mol
Reliability : (2) valid with restrictions
Accepted calculation method

14.12.2005

Media : water - air
Method : other (calculation)
Year :

Method : Estimated with HENRYWIN programme v3.10, US-EPA/Syracuse Research Corporation.
Result : Henry's Law Constant (HLC) =
4.11 E-08 atm.m3/mol
4.16 E-03 Pa.m3/mol
Test substance : Estimation from the molecular structure.
Reliability : (2) valid with restrictions
Accepted calculation method

14.12.2005

Media : other: water - organic carbon
Method : other (calculation)
Year :

Method : Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2005 ACD/Labs).
Result : Koc = 36320.92 at pH 1, 25 deg C
Koc = 11124.96 at pH 2, 25 deg C
Koc = 1414.97 at pH 3, 25 deg C
Koc = 159.11 at pH 4, 25 deg C
Koc = 29.79 at pH 5, 25 deg C
Koc = 16.82 at pH 6, 25 deg C
Koc = 15.52 at pH 7, 25 deg C
Koc = 15.39 at pH 8, 25 deg C
Koc = 15.38 at pH 9, 25 deg C
Koc = 15.38 at pH 10, 25 deg C
Test substance : Estimation from the molecular structure.
Reliability : (2) valid with restrictions
Accepted calculation method

14.12.2005

Media : other: water - organic carbon
Method : other (calculation)
Year :

Method : Estimated with PCKOC programme v1.66, US-EPA/Syracuse Research Corporation.
Result : Koc = 1.716 E+04
Log Koc = 4.24
Test substance : Estimation from the molecular structure.
Reliability : (2) valid with restrictions
Accepted calculation method

14.12.2005

Media : other: water - organic carbon
Method : other (calculation)
Year :

Method : Estimated from Log Kow = 2.67, with EPIWINWIN programme v3.12, Level III fugacity model, US-EPA/Syracuse Research Corporation.
Result : Koc = 192

Log Koc = 2.28

Reliability : (2) valid with restrictions
Accepted calculation method

09.12.2005

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : predominantly domestic sewage
Concentration : 100 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : 75 (±) % after 28 day(s)
Result : readily biodegradable
Kinetic of testsubst. : 8 day(s) = 33 %
14 day(s) = 67 %
20 day(s) = 73 %
%
%
Control substance : Aniline
Kinetic : 14 day(s) = 78 %
28 day(s) = 82 %
Deg. product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year : 1990
GLP : yes
Test substance : other TS

Test condition : The test substance, dissolved in a mineral medium, was inoculated with unadapted activated sludge (30 mg/l as dry solids), the oxygen consumption being measured automatically in a closed respirometer at 20 +/- 1 °C. Biodegradability is expressed as the percentage of oxygen consumption (corrected in the experiment by the oxygen consumption of a blank test) based on the theoretical oxygen consumption at 100 % mineralisation of 2385 mg O2/g test substance.
Test substance : Di-2-ethylhexyl phosphate, CAS No 298-07-7, purity not stated.
Reliability : (1) valid without restriction
Guideline study
Flag : Critical study for SIDS endpoint
14.12.2005 (18)

Type : aerobic
Inoculum : other
Concentration : 100 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : = 0 - 17 (±) % after 28 day(s)
Result :
Control substance : Aniline
Kinetic : %
%
Deg. product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year :
GLP : no data
Test substance : no data

Test condition : - Inoculum:
Sludge sampling were made at 10 different places in Japan: domestic and industrial sewage plants, rivers, lakes, bays.
Sludge concentration = 30 mg/l as suspended solids.

- Test solutions:
Abiotic control: 300 ml purified water containing 30 mg of test substance
Test substance assay: 300 ml inoculated test medium containing 30 mg test substance
Reference substance assay: 300 ml inoculated test medium containing 30 mg aniline
Control blank: 300 ml inoculated test medium

- Incubation temperature = 25 +/- 1 °C.

- Test vessels = 300 ml volume, closed, test solutions stirred by a magnetic stirrer

- Closed system oxygen consumption measuring apparatus (coulometer).

- % biodegradation by BOD.

Reliability : (2) valid with restrictions
Experimental data obtained at Chemicals Inspection and Testing Institute, JP, according to OECD guideline.

14.12.2005 (7)

Type : aerobic
Inoculum : predominantly domestic sewage
Contact time :
Degradation : 0 (±) % after 5 day(s)
Result :
Deg. product :
Method : OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year :
GLP :
Test substance :

Remark : related to BOD
Source : Bayer AG Leverkusen
Bayer Corporation Pittsburgh
Reliability : (4) not assignable
Primary source not retrieved.

14.12.2005 (8)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species : Cyprinus carpio (Fish, fresh water)
Exposure period : 42 day(s) at 25 °C
Concentration :
BCF : = 1.1 - 6
Elimination :
Method : OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year :
GLP : no data

Test substance	:	no data
Result	:	At 1 mg/l test substance concentration: BCF = 1.1 - 2.4 At 0.1 mg/l test substance concentration: BCF = 2.7 - 6.0
Test condition	:	Fish weight = about 30g Fish length = about 10 cm Fish lipid content = 4.7 % (average value) Feed = pelleted feed for carp, 2 % total body weight of test fish twice a day by halves, no feed supplied on the day of fish sampling Temperature controlled test water supplied continuously, at a rate of 200 - 800 ml/mn Temperature = 25 +/- 2 °C Concentration of dissolved oxygen in the test tank = 6 - 8 mg/l Number of fish at the initiation of exposure = 15 - 20 fish/level.
Reliability	:	(2) valid with restrictions Experimental data obtained at Chemicals Inspection and Testing Institute, JP, according to OECD guideline.

09.12.2005 (7)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 48 - 54
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	other TS
Result	:	96 h-LC50 = 49 - 56 mg/l (expressed as nominal concentrations) 96 h-LC50 = 48 - 54 mg/l (expressed as measured concentrations)
Test condition	:	Test organisms: Fish were obtained from a local hatchery which was supplied with soft lake water (pH about 7 and temperature about 11 °C), and transported (about 60 km) in plastic bags filled with water and oxygen. After arrival fish were acclimatised to the test water and test temperature (15 °C) for 6 days prior to the test. No food was given either during this period or during the toxicity test period (10 days). Fish body weight at the start of the test averaged 20g. Test water: Active charcoal filtered tap water, gently aerated at the test temperature for 3 days before addition of the test substance and the fish. Test vessels: Glass aquaria containing 50 l test water. Test solutions: The test substance was added directly to the aquaria and mixed for 1 mn with the test water by a commercial electric mixer. Test procedure: After mixing the test substance with the test water in the test vessels, the fish were immediately transferred from the acclimation tank to the test solutions by a dip net. 4 fish were used at each test concentration. During the entire test period the test solutions were gently aerated by the aid of an electric membrane pump, and maintained at a test temperature of 15 +/- 1 °C. Other bioassay procedure were according to "Standard Methods for Examination of Water and Wase Water" (APHA, 1971). Analytical monitoring: Total phosphorus determination was used to monitor the test substance concentrations in the test solutions. For this determination 1 ml of water sample was digested and the total phosphorus content determined spectrophotometrically. The accuracy of the method was considered to be +/- 2 % based on analysis of duplicate samples and standards.
Test substance	:	Di-(2-ethyl hexyl)-phosphoric acid from Bayer Chem. Co., Germany, purity not stated.
Reliability	:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment.
Flag	:	Critical study for SIDS endpoint

14.12.2005 (19)

Type	:	static
Species	:	Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	30
Limit test	:	
Analytical monitoring	:	no
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	other TS
Result	:	Result after 96 h exposure at 15 °C: 96 h-LC50 = 30 mg/l
Test condition	:	Test water : Local tap water (calcium concentration 18 mg/l) initially adjusted to pH 7.0 by sodium phosphate (final concentration 2.5 mM). Test solutions: The test substance was added to the test vessels from a stock solution in petroleum ether. The petroleum ether was evaporated just to dryness at room temperature before addition of 2 l of test water. Test procedure: At each concentration, 10 fry (average weight 0.15g) were exposed in a volume of 2 litres for at least 120 h. Tests were performed at preset temperatures of 5, 10, 15 and 20 °C. LC50 were determined at 24, 48, 96 and 120 h exposure by graphic estimation on log-probit paper.
Test substance	:	Di-(2-ethyl hexyl)-phosphoric acid from Bayer Chem. Co., Germany, purity not stated.
Reliability	:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment.
Flag	:	Critical study for SIDS endpoint

14.12.2005 (20)

Type	:	static
Species	:	Brachydanio rerio (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> 56
Limit test	:	
Analytical monitoring	:	no
Method	:	ISO 7346/1-3
Year	:	1975
GLP	:	no data
Test substance	:	other TS
Method	:	Exceptions to the ISO protocol: water temperature was kept at 25 degree C and the exposure period was extended to 144 hours (without renewal of toxicant).
Result	:	Exposure 24 hr 48 hr 144 hr LC50 (mg/l) >56.0 >56.0 >56.0
Test condition	:	Test water: Calcium (29.5 mg/l), Magnesium (7.5 mg/l), Sodium (56.5 mg/l), Bicarbonate (100.0 mg/l), Chloride (66.5 mg/l), Sulphate (56.0 mg/l), Nitrate (3.5 mg/l). The test water had a hardness of 100 mg/l expressed as $CaCO_3$, and an approximate initial pH of 8.3.

Test solutions:
The test substance solutions were prepared by pipetting into wide-mouthed Erlen-Meyer flasks (2 l) appropriate amounts (0-5.6 ml) of test substance stock solutions made up in acetone. After evaporation of the acetone just to dryness at room temperature, 1000 ml of premade aerated test water was added to each flask.
A solvent control (maximal amount of acetone evaporated just to dryness + 1000 ml of test water) and an ordinary control (1000 ml of test water) were included in the entire test procedure.
All solutions were allowed to stand over night at the test temperature (25 °C).

Test procedure:
On the following morning after test solution preparation, 5 juvenile zebrafish (average body weight 0.25g, previously held at 25°C and not fed for 48 h prior to use) were added at random to each flask.
Mortalities were recorded and dead fish were removed after 3, 6, 24, 48, 72, 96, 120 and 144 h.

Test substance : Di-(2-ethyl hexyl)-phosphoric acid from Bayer Chem. Co., Germany, purity not stated.

Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag : Critical study for SIDS endpoint

14.12.2005 (21)

Type : other: static or semi-static
Species : Oryzias latipes (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : = 148
Method : other
Year :
GLP : no data
Test substance : no data

Method : Japanese Industrial Standard JIS K 0102-1986-71 "Testing methods for industrial waste water".

Test condition : Test organisms:
Fish were obtained from a fish farm. Then fish were reared to flow through system for 3-5 weeks after external disinfection.
Fish were reared in an acclimatisation tank according to flow through system at a temperature of 25 +/- 2 °C for about 28 days. Abnormal fish were removed.

Test water:
Underground water.

Test vessels:
Round glass vessels containing 4 l of test water per concentration.

Test procedure:
10 fish/concentration
test temperature = 25 +/- 2 °C

Reliability : (2) valid with restrictions
Experimental data obtained at Chemicals Inspection and Testing Institute, JP, according to national guideline.

Flag : Critical study for SIDS endpoint

14.12.2005 (7)

Type : static
Species : Leuciscus idus (Fish, fresh water)

Exposure period	:	48 hour(s)
Unit	:	mg/l
LC0	:	20
LC100	:	40
Method	:	other: Bestimmung der akuten Wirkung von Stoffen auf Fische. Arbeitskreis "Fischtest" im Hauptausschuss "Detergentien" (15.10.73)
Year	:	
GLP	:	
Test substance	:	
Source	:	Bayer AG Leverkusen Bayer Corporation Pittsburgh
Reliability	:	(4) not assignable Primary source not retieved.

14.12.2005 (8)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 60.7
Analytical monitoring	:	no
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	no data
Result	:	Addition of acetone did not influence the LC50 values. EC50 values (with acetone): 48 h-EC50 = 60.7 mg/l (1 replicate) 72 h-EC50 = 35.7 mg/l (mean of 3 replicates) 96 h-EC50 = 19.7 mg/l (mean of 3 replicates) EC50 values (without acetone): 48 h-EC50 = 80.3 mg/l (mean of 2 replicates) 72 h-EC50 = 37.4 mg/l (mean of 3 replicates) 96 h-EC50 = 18.6 mg/l (mean of 3 replicates)
Test condition	:	Test organisms: Daphnia magna less than 66 hours old. Test procedure: Test temperature = 20 +/- 0.5 °C. Recorded pH at start and termination = 8.3 - 8.4 in controls, 8.0 - 8.1 in highest test concentration, 8.3 - 8.4 in lowest test concentration. Test performed in triplicates using 9 - 14 animals per concentration. Dead animals recorded after 3, 24, 48, 72 and 96 hours. LC50 and 95% confidence limits calculated using probit analysis. Other test procedures as in: Dave, G., Andersson K., Berglind R. and Hasselrot B. (1981). Toxicity of eight solvent extraction chemicals and of cadmium to water fleas, Daphnia magna, rainbow trout, Salmo gairdneri, and zebrafish, Brachydanio rerio, Comp. Biochem. Physiol., 69C (1): 83-98. Test solutions: An appropriate amount of test substance and 5 ml of deionised water were sonicated in a 10 ml vial for 30 s, diluted by test water and allowed to

equilibrate for one hour. Final test concentrations were prepared by diluting appropriate volumes of stock solution in test water up to 190 ml, and left for equilibrationfor 2 hours. The test animals were added in 10 ml of test water. In a parallele test, acetone was added to the test solutions at a final concentration of 500 µl/l. Exposures were initiated after equilibration for 3 h on addition of animals.

Test substance : Di-(2-ethyl hexyl)-phosphoric acid from Bayer Chem. Co., Germany, technical grade.

Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag : Critical study for SIDS endpoint

14.12.2005 (22)

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : > 42
Method : other
Year :
GLP : no data
Test substance : other TS

Result :

Exposure	24 hr	48 hr	72 hr	96 hr
LC50 (mg/l)	>42.0	>42.0	46.8	27.2
95% conf. limit			(19.8-110)	(9.6-77.2)

Test condition : Test water:
Modified Standard Reference water recommended by ISO (1977) : NaHCO3 (200 mg/l), K2SO4 (26 mg/l), K2HPO4 (6.8 mg/l), CaCl2.2H20 (297 mg/l);
The test water was prepared more than 24 hours in advance, aerated for 3 hours and allowed to stand over night. Just prior to use pH was adjusted to 7.8 by HCl addition.

Test vessels:
300 ml glass beakers (60 mm ID) covered with watch glasses.

Test solutions:
Stock solutions were made by dissolving weighed amounts of the test substance in acetone. One stock solution was made for each concentration in order to produce the desired nominal concentrations on addition of 50 µl stock solution to 200 ml test water.

Test procedure:
Before initiation of the test, the beakers were filled with 190 ml test water, followed by addition of 50 µl stock solution (50 µl acetone for the control), and the neonates (< 24 h old) pre-randomised in 10 ml test water. 12-15 animals were used for each test concentration/control. No food was added during the test.
Temperature: 20-23 degree C.
Illumination: diffuse light 12 hr per day.
Mortality was recorded after 3, 24, 48, 72 and 96 h. Other reactions of the animals and general activity were also recorded.
LC50 and 95% confidence limits were calculated with a log-probit analysis.
The Test was continued until mortality in controls reached 15% which occured between 48 and 120 h.

Test substance : Di-(2-ethyl hexyl)-phosphoric acid from Bayer Chem. Co., Germany, purity not stated.

Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag : Critical study for SIDS endpoint
14.12.2005 (21)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Chlorella emersonii (Algae)
Endpoint : growth rate
Exposure period : 72 hour(s)
Unit : mg/l
EC50 : > 100
Limit test :
Analytical monitoring : no
Method : other
Year :
GLP : no data
Test substance : other TS

Test condition : Test medium: mineral medium (Lorenzon H. In: Synchrony in cell division and growth, Zeuthen E. (Ed.), Interscience Publishers, NY, 1967, p 571.
Test solutions: The test substance was added from premade stock solutions in ethanol. The final concentration of ethanol in the test solutions (including controls) was 1/1000 (vol/vol).
Test concentrations: 50 and 100 mg/l
Aeration: 10 l/h air through the culture medium.
Temperature: 25+/- 0.5 °C.
Light: the cultures were continuously illuminated with cool white fluorescent tubes, giving a light intensity at the front surface of the culture tubes of 10 W/m2.
Inoculum: initial cell concentration corresponded to a chlorophyll concentration of 0.16 μg/ml.
Growth measurement: absorbance at 540 nm.
The exponential growth rates were determined from the linear part of the growth curves by means of linear regression analysis.

Test substance : Di-(2-ethyl hexyl)-phosphoric acid from Bayer Chem. Co., Germany, purity not stated.

Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag : Critical study for SIDS endpoint
14.12.2005 (20)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type :
Species : Pseudomonas fluorescens (Bacteria)
Exposure period : 24 hour(s)
Unit : mg/l
EC0 : 2340
Method : other
Year :
GLP : no data
Test substance : no data

Method : Inhibition of the growth of Pseudomonas fluorescens according to: Bestimmung der biologischen Schadwirkung toxischer Abwaesser gegen Bakterien. DEV, L 8 (1968) modified.

Result : No toxic effect at a dilution of the stock solution of 1:16 (2.5 g/l as Na salt = 2.34 g/l as anionic test substance).

Test condition : The test substance concentration in the stock solution was 4 % (40 g/l) as Na salt.
The test was carried out at 25 °C and at pH 7.
The test was performed for 24 hours in closed Kapsenberg tubes, and the culture growth was assessed optically.

Reliability : (2) valid with restrictions
Cited in peer reviewed secondary source. Performed according to national standard. Primary source not retrieved.

14.12.2005 (23) (2)

4.5.1 CHRONIC TOXICITY TO FISH

Species : Brachydanio rerio (Fish, fresh water)
Endpoint : other: survival of eggs and larvae
Exposure period : 10 day(s)
Unit : mg/l
Threshold conc. : = 21
Analytical monitoring : no
Method : other
Year :
GLP : no data
Test substance : other TS

Result : Embryo-larval Threshold Concentration = 21 mg/l

Test condition : Test organisms:
Eggs were collected approximately 5 hours after fertilisation. They were rinsed from fecal matters and viable eggs were transferred to Petri dishes containing the test substance in the test water.

Test water:
Calcium (29.5 mg/l), Magnesium (7.5 mg/l), Sodium (56.5 mg/l), Bicarbonate (100.0 mg/l), Chloride (66.5 mg/l), Sulphate (56.0 mg/l), Nitrate (3.5 mg/l).
The test water had a hardness of 100 mg/l expressed as $CaCO_3$, and an approximate initial pH of 8.3.

Test solutions:
Stock solutions of the test substance were made up with acetone. Appropriate volumes of the stock solutions were pipetted into the dishes and evaporated to dryness at room temperature. Control dishes were prepared by evaporating the greatest volume of acetone used in the test. Test water (50 ml) was then added to the dishes.

Test procedure:
10 - 15 viable eggs per dish were randomly distributed. New dishes were prepared every second day during the test and the survivors in each dish were transferred to the new dishes by the aid of a Pasteur pipette. Countings were performed daily and dead animals were removed in connection with the countings. The survival time recorded for each egg or larva is identical to the exposure time when each individual was found dead in connection with the counting.
The test was performed in a climate chamber at 25 °C with a 12 h light-dark photoperiod. No feeding of the test animals took place during the test which was terminated after 10 days.
Median survival times were plotted against nominal test concentrations on logarithmic scales and the threshold concentration value was obtained by interpolation.

Test substance : Di-(2-ethyl hexyl)-phosphoric acid from Bayer Chem. Co., Germany, purity not stated.

Reliability : (2) valid with restrictions

Meets generally accepted scientific standards, well documented and acceptable for assessment.

14.12.2005 (21)

Species : Oncorhynchus mykiss (Fish, fresh water)
Endpoint : other: survival of eggs and larvae
Exposure period : 48 day(s)
Unit : mg/l
Threshold conc. : = 20.6
Analytical monitoring : no
Method : other
Year :
GLP : no data
Test substance : other TS

Result : Embryo-larval Threshold Concentration = 20.6 mg/l
Test condition : Test organisms:
Eggs were bought from a local hatchery. They were eye-pointed at delivery and approximately 2 weeks were left before hatching. They were kept in a flow-through aquaria at 8 °C until the start of the test.

Test vessels:
Commercial jampots (diameter 75 mm, height 110 mm, total volume 360 ml)

Test water:
Calcium (29.5 mg/l), Magnesium (7.5 mg/l), Sodium (56.5 mg/l), Bicarbonate (100.0 mg/l), Chloride (66.5 mg/l), Sulphate (56.0 mg/l), Nitrate (3.5 mg/l).
The test water had a hardness of 100 mg/l expressed as CaCO3, and an approximate initial pH of 8.3.

Test solutions:
Stock solutions of the test substance were made up with acetone. Appropriate volumes of the stock solutions were pipetted into the test vessels and evaporated to dryness at room temperature. Control vessels were prepared by evaporating the greatest volume of acetone used in the test. Test water (250 ml) was then added to the test vessels and allowed to equilibrate during the night before embryos or larvae were introduced.

Test procedure:
Renewals of the test solutions were made every third to fourth day at the beginning, and every week at the end of the experimental period. Countings were performed daily and dead animals were removed in connection with the countings. The survival time recorded for each egg or larva is identical to the exposure time when each individual was found dead in connection with the counting.
The test was performed at 8 +/- 1 °C with a 12 h light-dark photoperiod. No feeding of the test animals took place during the test which was terminated 48 days after hatching.
Median survival times were plotted against nominal test concentrations on logarithmic scales and the threshold concentration value was obtained by interpolation.

Test substance : Di-(2-ethyl hexyl)-phosphoric acid from Bayer Chem. Co., Germany, purity not stated.

Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

14.12.2005 (21)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

In Vitro/in vivo : In vivo
Type : Metabolism
Species : rat
Number of animals
Males : 12
Females :
Doses
Males : 0.25, 0.1, 3.0% w/w in diet
Females :
Vehicle :
Route of administration : oral feed
Exposure time : 5 day(s)
Product type guidance :
Decision on results on acute tox. tests :
Adverse effects on prolonged exposure :
Half-lives : 1st:
2nd:
3rd:
Toxic behaviour :
Deg. product :
Method :
Year : 1987
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : The authors commented that both di(2-ethylhexyl)phthalate and 2-ethylhexylhexanoic acid share the properties of induction of xenobiotic-metabolising enzymes and/or proliferation of peroxisomes and/or mitochondria as well as the 2-ethylhexyl group. They postulated that all three substances may be converted metabolically to the same inducer and/or proliferator. They did not name this proposed metabolite, but a review of the study (ECETOC, 1992) presumed this to be 2-ethylhexanol.

Result : Using a standard conversion factor 1/10 to convert dose (ppm diet) to dose (mg/kg/day) for young rats, approximate doses for each test group were:

0.25% 250 mg/kg/day
1.0% 1000 mg/kg/day
3.0% 3000 mg/kg/day

Significant increases were reported in several hepatic enzymes for rats receiving the 1% or 3% diets:

Cytosolic epoxide hydrolase activity was increased approximately 3.3-fold at both 1% and 3%.

Total cytochrome P-450 was increased 2-fold (1%) and 3-fold (3%). There was no increase in cytochrome P-450c, but cytochromes P450b+e were induced 20-fold (1%) and 35-fold (3%).

Smaller effects were observed on NADPH-cytochrome c reductase, microsomal epoxide hydrolase and microsomal cytochrome b5.

There was no effect on cytosolic glutathione transferase activity.

A 28-fold increase in cyanide-insensitive palmitoyl-CoA oxidation and a 4-fold increase of the total mitochondrial protein, with smaller increases in total catalase and cytochrome oxidase activities, were observed, indicating

that the test substance causes proliferation chiefly of peroxisomes but also mitochondria in rat liver.

Test condition : The test substance was administered to male Sprague-Dawley rats, 3 per group, for 5 days at 0.25, 1.0 and 3.0% (2,500, 10,000 and 30,000 ppm) w/w in the diet.

For full details, see Section 5.4, 5-day subacute study.

Reliability : (4) not assignable
Insufficient experimental detail is available to assign reliability.

14.12.2005 (24) (25)

In Vitro/in vivo : In vivo
Type : Metabolism
Species : mouse
Number of animals
Males :
Females :
Doses
Males : 1.0% w/w diet
Females :
Vehicle :
Route of administration : oral feed
Exposure time :
Product type guidance :
Decision on results on acute tox. tests :
Adverse effects on prolonged exposure :
Half-lives : 1st:
2nd:
3rd:
Toxic behaviour :
Deg. product :

Result : Using a standard conversion factor 1/5 to convert dose (ppm diet) to dose (mg/kg/day) for young mice, the dose of 1.0% in the diet approximated to a dose of 2000 mg/kg bw.

An approximately 3-fold induction of cytosolic epoxide hydrolase and a 2-fold induction of microsomal epoxide hydrolase was reported. The increase in specific activity of hepatic cytosolic epoxide hydrolase reflected a corresponding increase in enzyme protein, as determined immunochemically.

Test condition : The test substance was administered to male 20-22 g C57BL/6 mice at 1% (10,000 ppm) w/w in the diet. Subcellular fractionisation of liver homogenates was performed and the specific activity of hepatic cytosolic and microsomal epoxide hydrolase activity was measured.

Reliability : (4) not assignable
Insufficient experimental detail is available to assign reliability.

14.12.2005 (24) (26)

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : = 1400 mg/kg bw
Species : rat
Strain : Wistar
Sex : male/female
Number of animals : 50
Vehicle : other: none
Doses : 500, 880, 1260, 2000, 3000 mg/kg bw
Method : other

Year : 1977
GLP : no data
Test substance : other TS

Result : Mortality:

Dose	m	f
500	1/5	0/5
880	0/5	1/5
1260	2/5	2/5
2000	1/5	4/5
3000	5/5	5/5

Signs of toxicity:
Slight to severe depression, death.
No gross pathological alterations clearly related to exposure were noted in animals dying during the study or in survivors.
LD50 was calculated as 1400 (1090-1790) mg/kg bw

Test condition : Groups of ten (5m:5f) Albino rats, 150-300g were maintained under laboratory conditions for 7 days then fasted overnight. Rats were dosed individually by gavage. Test material was administered as received (specific gravity 0.88), up to the top dose feasible of 40 ml/kg. Animals were observed for signs of pharmacological activity and toxicity at 1, 3, 6 and 24 hours, then daily to a total of 14 days. Initial and final body weights, mortalities and reactions were recorded. Necropsy was carried out on animals sacrificed at the end of the 14-day observation period.

Test substance : Di (2-Ethylhexyl) Phosphoric Acid (DEHPA) Lot H11090677, purity not given.

Reliability : (2) valid with restrictions
Comparable to guideline study.

Flag : Critical study for SIDS endpoint

08.12.2005 (27)

Type : LD50
Value : = 500 - 5000 mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 20
Vehicle : other: none
Doses : 500, 5000 mg/kg bw
Method : other: no data
Year : 1982
GLP : no data
Test substance : other TS

Result : All animals dosed at 5 g/kg were found dead within 24 hours after dosing. All animals of the lower dose group of 0.5 g/kg survived 14 days. Necropsy findings of high dose decedents included severely reddened abdominal walls, enlarged blood vessels and reddened lining of the gastrointestinal tract. The stomach lining was a very dark red-black color. Adrenals and pancreas were reddened in the majority of animals. Lungs in most instances were found to be scarlet red. Kidneys were pale and thymus darkened.

Low dose animals gained weight throughout the study. Clinically the animals exhibited oral/nasal discharge and diarrhea on the day of dosing only.

The oral LD50 was judged to be betewwn 500 mg/kg and 5 g/kg.

Test condition : Two groups of 5 male and 5 female fasted Sprague-Dawley rats were dosed once by oral gavage with the liquid test material at dose levels of 5 g/kg and 0.5 g/kg. They were observed frequently on the day of treatment

and daily thereafter for 14 days.

Animals which died during the observation period were necropsied. Surviving animals were weighed on days 0, 7 and 14, then killed and discarded.

Test substance : Bis (2-Ethylhexyl) Phosphoric Acid (DEHPA) Lot #091010TC49929 DR, purity not given.

Reliability : (2) valid with restrictions
Short report of study comparable to guideline study.

23.11.2005 (28)

Type : LD50
Value : = 4.94 ml/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: no data
Year :
GLP : no data
Test substance : no data

Result : Oral Rat LD50 4940 uL/kg. Equivalent to 4742 mg/kg (density = 0.96 g/ml).

Reliability : (4) not assignable
Union Carbide MSDS, source of RTECS citation, not available for verification.

08.12.2005 (29)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > 2000 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 6
Vehicle : other: none
Doses : 2.0 g/kg
Method : other: no data
Year : 1982
GLP : no data
Test substance : other TS

Result : There were no deaths and no significant changes in bodyweight after 14 days. Bodyweights at day 7 were slightly depressed. No clinical signs of toxicity were observed.

The test material elicited signs of severe dermal irritation in all animals. Eschar and severe edema were observed and persisted through the study.

Test condition : The hair was clipped from the entire trunk of 3 male and three female rabbits. The skin of 3 animals (2 male, 1 female) was abraded, while the skin of the remaining 3 animals remained intact. The liquid test substance was administered at a dose level of 2.0 g/kg and the trunk of each animal

covered in gauze and an occlusive rubber dam. The animals were observed for signs of toxicity frequently on the day of treatment. After 24 hours the rabbits were unwrapped and the test sites wiped with cotton wetted with physiological saline. The animals were observed for signs of toxicity daily thereafter for 14 days. The test sites were assessed for irritation at 24 and 72 hours, then 7, 10 and 14 days after treatment. After 14 days the surviving animals were killed and discarded.

Test substance : Bis (2-Ethylhexyl) Phosph0ric Acid (DEHPA) Lot #091010TC49929 DR, purity not given.

Reliability : (2) valid with restrictions
Short report, comparable to guideline study.

Flag : Critical study for SIDS endpoint

08.12.2005 (30)

Type : LD50
Value : = 1.25 ml/kg bw
Species : rabbit
Strain : no data
Sex : no data
Number of animals :
Vehicle :
Doses :
Method : other: no data
Year : 1972
GLP : no data
Test substance : other TS

Result : Dermal Rabbit LD50 1250 uL/kg. Equivalent to 1200 mg/kg (density = 0.96 g/ml).

Reliability : (4) not assignable
Union Carbide MSDS, source of RTECS citation, not available for assessment.

08.12.2005 (29)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : LD50
Value : 50 - 100 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Route of admin. : i.p.
Exposure time :

Source : Bayer AG Leverkusen
Bayer Corporation Pittsburgh

Reliability : (4) not assignable

08.12.2005 (31)

Type : LDLo
Value : 63 mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :

Route of admin. : i.p.
Exposure time :

08.12.2005 (32)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 6
Vehicle : other: none
PDII : 6.2
Result : highly irritating
Classification : irritating
Method : Draize Test
Year : 1982
GLP : no data
Test substance : other TS

Result : Mean Score
Intact skin:
Erythema
24 h: 3.2
72 h: 3.3
Oedema:
24 h: 3.3
72 h: 2.3

Abraded skin:
Erythema
24 h: 3.2
72 h: 3.7
Oedema:
24 h: 3.5
72 h: 2.3

PDII: 6.2

Skin irritation showed little improvement at 72 hours. Eschar formation was observed to be present at all test sites at day 7 and in 4 of 12 sites after 14 days. Abrasion of the test sites did not result in increased irritation. DEHPA was determined to be a severe skin irritant.

Test condition : The hair was clipped from the sides and backs of 6 New Zealand White rabbits. One test site was prepared on each side of each rabbit. The skin at one site of each was abraded. 0.5 ml of the test material was applied to each test site under patches secured by gauze and tape and rubber dam. After 24 hours the wrapping was removed and the test sides washed with physiological saline. The test sites were evaluated for irritation 2 hours later and again at 72 hours, and 7 and 14 days.

Test substance : Bis (2-Ethylhexyl) Phosphite (DEHPA) Lot #091010TC49929 DR, purity not given.

Reliability : (2) valid with restrictions
Short report, comparable to guideline study.

Flag : Critical study for SIDS endpoint

13.12.2005 (33)

Species : rabbit
Concentration : undiluted

Exposure : Occlusive
Exposure time : 48 hour(s)
Number of animals : 6
Vehicle : other: none
PDII : 4.85
Result : irritating
Classification : irritating
Method : other
Year : 1977
GLP : no data
Test substance : other TS

Method : Test for dermal corrosion according to 49CFR 173.240 (a)(1).
Result : Mean Score
Intact skin:
Erythema
4 h: 1.0
48 h: 2.2
Oedema:
4 h: 3.7
48h: 2.8

Subtotal: 9.7
PDII: 4.85

Test sites for all animals were blanched at 4 hours but had recovered at the 48 hour observation. No permanent damage was noted. The test substance was not corrosive.
Source : Rhodia Consumer Specialties LTD Oldbury, West Midlands
Test condition : Six rabbits, 3 male, 3 female, each non-abraded, received 0.5 ml single application under an occluded patch. Observations were made at 4 and 48 hours.
Test substance : Bis (2-Ethylhexyl) Phosphite (DEHPA) Lot #11090677, purity not given
Reliability : (2) valid with restrictions
Short report. Comparable to guideline study.

13.12.2005 (34)

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 6
Vehicle : other: none
PDII : 0
Result : not irritating
Classification : not irritating
Method : other
Year : 1971
GLP : no data
Test substance : other TS

Method : Comparable to Federal Register, Vol 26, No 155, p 7336, 12 August 1961
Result : Mean Score
Intact skin:
Erythema
4 h: 0
48 h: 0
Oedema:
4 h: 0
48h: 0
Subtotal: 0
PDII: 0

The test substance was not irritant

Source : Rhodia Consumer Specialties LTD Oldbury, West Midlands

Test condition : Prior to the dermal applications, the hair was clipped from a wide area of 6 male albino rabbits. One side of the back of each was abraded, while the other side was left intact. 0.5 ml of undiluted test material was applied to each of the test sites. The test sites were occluded with gauze patches and the rabbits wrapped with rubber damming. The damming and gauze were removed after 24 hours and the test sites were examined and scored for erythema, oedema and eschar formation. The sites were examined again after 72 hours and the primary dermal irritation index was calculated.

Test substance : Bis (2-Ethylhexyl) Phosphite (DEHPA), purity not given

Reliability : (2) valid with restrictions
Short report. Comparable to guideline study, but no information available on substance purity.

Flag : Critical study for SIDS endpoint

13.12.2005 (35)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : corrosive
Classification :
Method : other: see remarks
Year : 1978
GLP :
Test substance :

Remark : 2 animals, 500 ul/animal, 1-8 h exposure time, post exposure time 7 d

Source : Bayer AG Leverkusen
Bayer Corporation Pittsburgh

Reliability : (4) not assignable

13.12.2005 (36)

Species : rabbit
Concentration : 5 mg
Exposure :
Exposure time : 24 hour(s)
Number of animals :
Vehicle :
PDII :
Result : highly irritating
Classification : irritating
Method :
Year : 1986
GLP :
Test substance :

Remark : Reported as causing severe irritation in two secondary references (RTECS, Sax), but mild irritation in a third (DOSE).

Reliability : (4) not assignable

13.12.2005 (37)

Species : other: no data
Concentration :
Exposure :
Exposure time :

Number of animals :
Vehicle :
PDII :
Result : corrosive
Classification :
Method : other: no data
Year :
GLP :
Test substance :

Remark : Stated to be a "DOT corrosive material".
Source : Bayer AG Leverkusen
Bayer Corporation Pittsburgh
Reliability : (4) not assignable
Not assignable. Secondary reference with no primary reference shown.
13.12.2005 (38)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : .1 ml
Exposure time : 72 hour(s)
Comment :
Number of animals : 6
Vehicle : none
Result : corrosive
Classification : risk of serious damage to eyes
Method : other
Year : 1971
GLP : no data
Test substance : other TS

Method : According to Federal Register Vol. 29, No. 162, p. 13009, 17 September 1964
Result :

Mean Scores	1	2	3	4	5	6	7 (days)
Cornea:	73.3	73.3	76.7	76.6	73.3	73.3	73.3
Iris:	9.2	9.2	10	10	10	10	10
Conjunctiva:	17.3	18	18.3	16.3	15.3	15.3	15
Total:	99.8	100.5	105	103	98.7	98.7	98.3

Source : Rhodia Consumer Specialties LTD Oldbury, West Midlands
Test condition : 6 New Zealand albino rabbits were used in the study. 0.1 ml of undiluted test material was instilled into the right eye of each rabbit with the untreated eye serving as a control. The treated eyes remained unwashed. The treated eyes were examined daily for 7 days following instillation of the test material. Ocular reactions were graded.
Test substance : Bis (2-Ethylhexyl) Phosphite (DEHPA), purity not given
Reliability : (2) valid with restrictions
Short report of test comparable to guideline study.
Flag : Critical study for SIDS endpoint
22.11.2005 (39)

Species : rabbit
Concentration : undiluted
Dose : .1 ml
Exposure time : 72 hour(s)
Comment :
Number of animals : 6
Vehicle : none
Result : highly irritating

Classification : irritating
Method : other: no data
Year : 1982
GLP : no data
Test substance : other TS

Result : Mean Irritation Scores:

Washed Eyes:

Mean Scores	1h	24h	48h	72h	
Cornea:		20.0	21.7	13.3	13.3
Iris:	1.7	3.3	3.3	5.0	
Conjunctiva:	14.0	19.3	18.7	20.0	
Total:	35.7	44.3	35.3	38.3	

Unwashed Eyes:

Mean Scores	1h	24h	48h	72h	
Cornea:		28.3	21.7	13.3	15.0
Iris:	1.7	5.0	6.0	5.0	
Conjunctiva:	12.7	20.0	12.0	20.0	
Total:	42.7	46.7	35.3	40.0	

Corneal opacity was still present after 14 days in five of the six animals tested. The test material is a strong irritant and washing did not reduce the irritation.

Test condition : 6 New Zealand albino rabbits were used in the study. 0.1 ml of undiluted test material was instilled into one eye of each rabbit with the untreated eye serving as a control. Three treated eyes remained unwashed, the other three were washed for one miniute with warm water, 20 seconds after instillation. The treated eyes were scored for irritation at 1, 24, 48 and 72 hours after treatment. days following instillation of the test material. Ocular reactions were graded.

Test substance : Bis (2-Ethylhexyl) Phosphite (DEHPA) Lot #091010TC49929 DR, purity not given.

Reliability : (2) valid with restrictions
Short report, comparable to guideline study

22.11.2005 (40)

Species : rabbit
Concentration :
Dose :
Exposure time :
Comment :
Number of animals :
Vehicle :
Result : corrosive
Classification :
Method : other: see remarks
Year :
GLP :
Test substance :

Remark : 2 animals, 100ul/animal, post exposure time 7 d;
Source : Bayer AG Leverkusen
Bayer Corporation Pittsburgh

22.10.2001 (36)

Species : rabbit
Concentration :
Dose : 250 other: ug
Exposure time : 24 hour(s)
Comment :
Number of animals :

Vehicle	:	
Result	:	highly irritating
Classification	:	risk of serious damage to eyes
Method	:	
Year	:	1986
GLP	:	
Test substance	:	
Remark	:	Reported as causing severe irritation in secondary references.
Reliability	:	(4) not assignable

13.12.2005 (37)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-acute
Species	:	rat
Sex	:	male
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	5 days
Frequency of treatm.	:	Daily
Post exposure period	:	
Doses	:	0.25, 1.0 and 3.0% w/w diet
Control group	:	yes, concurrent no treatment
NOAEL	:	= 2500 ppm
Method	:	
Year	:	1987
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Result : Using a standard conversion factor 1/10 to convert dose (ppm diet) to dose (mg/kg/day) for young rats, approximate doses for each test group were:

0.25%	2500 ppm	250 mg/kg/day
1.0%	10000 ppm	1000 mg/kg/day
3.0%	30000 ppm	3000 mg/kg/day

There were no obvious signs of toxicity and no effect on bodyweight gain. No full evaluation of standard toxicity endpoints was reported.

Effects on hepatic enzyme induction, statistically significant at 1.0 and 3.0% in diet, are reported in Section 5.0, Metabolism.

NOAEL: 0.25% in diet (approx. 250 mg/kg bw/day)

Test condition : The test substance was dissolved in 20 ml acetone and mixed with 100 g powdered rat chow, dried for 12 to 24 hours and then stored at -20 deg C.

Test substance was administered to male Sprague-Dawley rats, 3 per group, for 5 days at 0.25, 1.0 and 3.0% (2,500, 10,000 and 30,000 ppm) w/w in the diet. A group of 3 control rats was fed untreated R3 pellets. The rats consumed approximately 10 g of diet per day.

At the end of the treatment period, the rats were starved overnight to reduce hepatic levels of glycogen before decapitation. The liver was immediately removed, weighed and homogenised for assessment of hepatic enzyme induction.

Rats were observed for signs of toxicity and were weighed at the start of the study and at terminaton. No full necropsy or histopathological examination was reported.

Reliability : (4) not assignable
Insufficient experimental detail is available to assign reliability.

13.12.2005 (25)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium TA-1535, TA-1537, TA-1538, TA-98, TA-100, Saccharomyces cerevisiae D4
Test concentration : 0.001ul to 5ul per plate
Cycotoxic concentr. : 5 ul/plate
Metabolic activation : with and without
Result : negative
Method : other
Year : 1977
GLP : no data
Test substance : other TS

Result : No dose-related increases in revertant colonies were observed with any strain, with or without activation.

Slight toxicity was observed at 5 ul/plate with strains TA-1357, TA-1358, TA-98 and TA-100, with and without activation.

Source : Rhodia Consumer Specialties LTD Oldbury, West Midlands
Test condition : The test compound was examined for mutagenic activity in the presence and absence of liver microsomal enzyme preparations from Aroclor-induced rats. Acetone was used as a solvent. Concentrations evaluated were 0.001, 0.01, 0.1, 1.0 and 5.0 ul/plate. Positive controls were used to confirm the validity of the test.
Test substance : Bis (2-Ethylhexyl) Phosphite (DEHPA) Lot #11090677, purity not given.
Reliability : (2) valid with restrictions
Comparable to test guideline, using approved strains of S. typhimurium. Current guidelines would require in addition either E.coli WP2 strains or S. typhimurium TA102, however this omission is not considered critical.
Flag : Critical study for SIDS endpoint

23.11.2005 (41)

Type : Ames test
System of testing : S. typhimurium TA 98, TA100, TA 1535, TA1537
Test concentration : 4 - 2500 ug/plate
Cycotoxic concentr. : 100 ug/plate
Metabolic activation : with and without
Result : negative
Method : other: no data
Year : 1982
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Doses up to 20 mg per plate did not lead to bacteriotoxic effects. The total bacteria counts remained unchanged. Growth inhibition was not observed. The substance revealed only weak strain-specific bacteriotoxic effects in the given dose range with and without S-9 Mix, so that this range was acceptable for assessment purposes.

There were no indications of any mutagenic effect from di-2-ethylhexyl phosphate. Neither a dose-dependent doubling nor a biologically-relevant

increase in the number of mutations compared to the negative controls was ascertained.

The positive controls Endoxane, Trypaflavine and 2-aminoanthracene clearly were mutagens, eliciting a biologically-relevant increase in the number of mutations compared to the negative controls

Source : Bayer AG Leverkusen
Bayer Corporation Pittsburgh

Test condition : The test compound was examined for mutagenic activity in the presence and absence of liver microsomal enzyme preparations from Aroclor-induced rats. DMSO was used as a solvent. Concentrations evaluated were 4, 20, 100, 500 and 2500 ug/plate. Positive controls Endoxane, Trypaflavine and 2-aminoanthracene were used to confirm the validity of the test.

Reliability : (2) valid with restrictions
Comparable to test guideline, using approved strains of S. typhimurium. Current guidelines would require in addition either E.coli WP2 strains or S. typhimurium TA102, however this omission is not considered critical.

Flag : Critical study for SIDS endpoint
23.11.2005 (42)

Type : Mouse lymphoma assay
System of testing : L5178Y/TK+/- mouse lymphoma cells
Test concentration : 0.06 to 0.9 µl/ml without metabolic activation and 0.05 to 0.085 µl/ml with S9 activation.
Cycotoxic concentr. : 1.0 µl/ml
Metabolic activation : with and without
Result : negative
Method : other
Year : 1982
GLP : no data
Test substance : other TS

Result : None of the treated clonable cultures exhibited mutant frequencies which were significantly different from those of solvent-treated controls, either with or without metabolic activation.
The total growth ranged from 2% to 118% of solvent-treated controls for non-activated cultures and from 4% to 193% for activated cultures. Total growth was dependent upon the applied concentration of the test substance for both activated and non-ctivated cultures.

Source : Rhodia Consumer Specialties LTD Oldbury, West Midlands

Test condition : The test compound was examined directly and in the presence of liver microsomal enzyme preparations from Aroclor-induced rats. Dimethylsulphoxide was used as a solvent. Concentrations evaluated were 0.06, 0.065, 0.07, 0.075, 0.08, 0.085 and 0.09 ul/ml for non-activated cultures and 0.05, 0.055, 0.06, 0.065, 0.07, 0.075, 0.08 and 0.085 ul/ml for activated cultures. Positive controls were used to confirm the validity of the test.

Test substance : Bis (2-Ethylhexyl) Phosphite (DEHPA) Lot 04291301, purity not given.

Reliability : (2) valid with restrictions
Comparable to guideline study, but with no indication whether study was conducted according to GLP.

Flag : Critical study for SIDS endpoint
22.11.2005 (43)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

08.12.2005

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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(43) Blackburn GR, 1982, Evaluation of the Mutagenic Potential of Di (2-Ethylhexyl) Phosphoric Acid in the Mouse Lymphoma (L578Y TK+/-) Mutagenesis Assay, Study No.:11221, Mobil Environmental & Health Science Laboratory, Plainsboro, NJ. Mobil Chemical Company Internal Report 1221-81 (unpublished report).

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-16174B

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I U C L I D

D a t a S e t

Existing Chemical	ID: 78-42-2
CAS No.	78-42-2
EINECS Name	tris(2-ethylhexyl) phosphate
EINECS No.	201-116-6
TSCA Name	Phosphoric acid, tris(2-ethylhexyl) ester
Molecular Formula	C24H51O4P

Producer Related Part
Company:
Creation date: 15-JUL-1999

Substance Related Part
Company:
Creation date: 15-JUL-1999

Memo: Phosphoric Acid Derivatives Panel

Printing date: 28-NOV-2001
Revision date:
Date of last Update: 28-NOV-2001

Number of Pages: 34

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: American Chemistry Council (formerly Chemical Manufacturers Association) Phosphoric Acid Derivatives Panel
Street: Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States
Phone: 703-741-5600
Telefax: 703-741-6091

16-OCT-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

16-OCT-2001

Type: cooperating company
Name: Baker Petrolite Corporation
Country: United States

16-OCT-2001

Type: cooperating company
Name: Crompton Corporation
Country: United States

16-OCT-2001

Type: cooperating company
Name: ICI Americas (Uniqema)
Country: United States

16-OCT-2001

Type: cooperating company
Name: Noveon, Inc. (formerly BF Goodrich)
Country: United States

16-OCT-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information
-

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms
-

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern
-

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value: 87 degree C
Method: other: MPBPWIN Program, version 1.31
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 146.94 deg C (Gold and Ogle Method)
Mean Melt Pt : 110.97 deg C (Joback; Gold,Ogle Methods)
Selected MP: 86.99 deg C (Weighted Value)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
27-JUN-2001 (1)

Value: < -70 degree C
Source: Bayer AG Leverkusen
12-AUG-1992 (2)

2.2 Boiling Point

Value: 446.3 degree C at 1013 hPa
Method: other: MPBPWIN Program, version 1.31
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Boiling Point: 446.31 deg C (Adapted Stein and Brown Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
22-OCT-2001 (1)

Value: ca. 210 degree C at 5 hPa
Source: Bayer AG Leverkusen
12-AUG-1992 (2)

2.3 Density

Type: density
Value: .92 g/cm3 at 20 degree C
Source: Bayer AG Leverkusen
12-AUG-1992 (2)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: .000000205 hPa at 25 degree C
Method: other (calculated): MPBPWIN Program, version 1.31
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 446.31 deg C (estimated))
(Using MP: 86.99 deg C (estimated))
VP: 1.17E-008 mm Hg (Antoine Method)
VP: 1.54E-007 mm Hg (Modified Grain Method)
VP: 3.11E-007 mm Hg (Mackay Method)
Selected VP: 1.54E-007 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
16-OCT-2001 (1)

Value: < .01 hPa at 20 degree C
Source: Bayer AG Leverkusen
12-AUG-1992 (2)

2.5 Partition Coefficient

log Pow: 4.2
Method: other (measured): according to Saeger et al. (1979)
Year: 1979
GLP: no data
Testsubstance: other TS: tris(2-ethylhexyl)phosphate; obtained from FMC Corporation; purity > 90%
Result: octanol/water partition coefficient = 16,800
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
22-OCT-2001 (3)

log Pow: 4.1
Method:
Year:
Source: Bayer AG Leverkusen
16-OCT-2001 (4)

log Pow: .7
Method: other (calculated): Leo, A.: CLOGP-3.54 MedChem Software 1989. Daylight, Chemical Information Systems, Claremont, CA 91711, USA
Year:
Source: Bayer AG Leverkusen
12-AUG-1992 (5)

log Pow: .8
Method:
Year:
Remark: experimentally determined
Source: Bayer AG Leverkusen
21-SEP-1992 (6)

log Pow: 9.491
Method: other (calculated): KOWWIN Program, version 1.65
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
16-OCT-2001 (1)

2.6.1 Water Solubility

Value: 2 mg/l
Method: other
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
16-OCT-2001 (7)

Value: .00001 mg/l at 25 degree C
Method: other: WSKOW Program, version 1.36
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
16-OCT-2001 (1)

Value: < .1 g/l at 20 degree C
Source: Bayer AG Leverkusen
16-OCT-2001 (2)

Value: 1000 other: ppm
Method: other: according to Saeger et al. (1979)
GLP: no data
Testsubstance: other TS: tris(2-ethylhexyl)phosphate; obtained from FMC Corporation; purity > 90%
Remark: The true solubility of TEHP is probably less than 1000 ppm, The compound turned cloudy when shaken with water, suggesting the formation of an emulsion or a decomposition product.
22-OCT-2001 (3)

2.6.2 Surface Tension
-

2.7 Flash Point

Value:	> 170 degree C
Type:	other
Method:	other: DIN 51376
Year:	
Source:	Bayer AG Leverkusen

12-AUG-1992 (2)

2.8 Auto Flammability

-

2.9 Flammability

-

2.10 Explosive Properties

-

2.11 Oxidizing Properties

-

2.12 Additional Remarks

-

3.1.1 Photodegradation

```
Type:              air
INDIRECT PHOTOLYSIS
  Sensitizer:      OH
  Conc. of sens.:  1560000 molecule/cm3
  Rate constant:   .000000000097 cm3/(molecule * sec)
  Degradation:     50 % after 1.3 hour(s)
Method:            other (calculated): AOP Program (v1.89)
  Year:            1999                          GLP: no
Test substance:    other TS: molecular structure
Result:            ------- SUMMARY (AOP v1.89): HYDROXYL RADICALS --------------
                   Hydrogen Abstraction       =  97.8576 E-12 cm3/molecule-sec
                   Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
                   Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
                   Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
                   Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
                   Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

                      OVERALL OH Rate Constant =  97.8576 E-12 cm3/molecule-sec
                      HALF-LIFE =     0.109 Days (12-hr day; 1.5E6 OH/cm3)
                      HALF-LIFE =     1.312 Hrs
Reliability:       (2)  valid with restrictions
                   Accepted calculation method
Flag:              Critical study for SIDS endpoint
27-JUN-2001                                                                    (1)

Type:
Method:
  Year:                                          GLP:
Test substance:
Result:            ca. 80 % degradation by UV-light (1h)
Source:            Bayer AG  Leverkusen
Flag:              Critical study for SIDS endpoint
26-NOV-1992                                                                    (4)
```

3.1.2 Stability in Water

Remark: An attempt to make a water solution of Phosphoric acid, 2-ethylhexyl ester demonstrated that the product was obviously water insoluble and prevented a determination of hydrolysis. (See IUCLID on CASRN 12645-31-7)

3.1.3 Stability in Soil

-

3.2 Monitoring Data (Environment)

-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - water - soil - sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: Level III Fugacity Model
Year:
Result:

Media	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.312	2.62	1000	7.59e-013
Water	10.9	208	1000	5.02e-017
Soil	31.2	208	1000	1.08e-019
Sediment	57.6	832	0	9e-018

Persistence Time: 350 hr
Reaction Time: 370 hr
Advection Time: 6.6e+003 hr
Percent Reacted: 94.7
Percent Advected: 5.3

Remark: Default input values of 1000 kg/hr were used for model.
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
16-OCT-2001 (1)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: predominantly domestic sewage
Degradation: 0 % after 28 day
Result: under test conditions no biodegradation observed
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1982 GLP: no
Test substance: other TS
Remark: related to BOD
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
22-OCT-2001 (8)

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Degradation: 0 % after 28 day
Result: under test conditions no biodegradation observed
Method:
Year: GLP:
Test substance:
Remark: Method:
"Biodegradation test of chemical substance by micro-organisms etc." stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "301C, Ready Biodegradability: Modified MITI Test I" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
related to BOD
sludge conc.: 30 mg/l
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
22-OCT-2001 (7)

Type: aerobic
Inoculum: activated sludge, domestic
Degradation: 20% ±8% after 238 day
Method: other: SCAS-Test; EEC Directive 79/831 Annex V Part C
Year: GLP: no data
Test substance: other TS: tris(2-ethylhexyl)phosphate; obtained from FMC Corporation; purity > 90%
Test condition: Concentration: 3 mg/l/24 h
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
22-OCT-2001 (3)

Type: aerobic
Inoculum: activated sludge
Degradation: 55 % after 2 day
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
27-JAN-1994 (4)

Type: aerobic
Inoculum: other: activated sludge, after acclimatization
Degradation: 60 % after 2 day
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
27-JAN-1994 (4)

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day
Concentration: 2 mg/l
BCF: 2.4 - 6.5
Elimination:
Method: OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year: 1981 GLP:
Test substance:
Remark: log Pow: 5.04
% lipid average: 5.1
Method: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
Source: Bayer AG Leverkusen
22-OCT-2001 (7)

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day
Concentration: .2 mg/l
BCF: 9.2 - 22
Elimination:
Method: OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year: 1981 GLP:
Test substance:
Remark: log Pow: 5.04
% lipid aaverage: 5.1
Method: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree f Bioconcen-

tration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).

Source: Bayer AG Leverkusen
22-OCT-2001 (7)

Species: other
Exposure period:
Concentration:
BCF: 3.16
Elimination:
Method: other: BCF Program (v2.13)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Result: CHEM : Phosphoric acid, tris(2-ethylhexyl) ester
MOL FOR: C24 H51 O4 P1
MOL WT : 434.65
---------- Bcfwin v2.12 ----------
Log Kow (estimated) : 9.49
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 9.49

Equation Used to Make BCF estimate:
Log BCF = -1.37 log Kow + 14.4 + Correction

Correction(s):	Value
Phosphate ester	-0.780
Alkyl chains (8+ -CH2- groups)	-1.500

Minimum Log BCF of 0.50 applied when Log Kow > 7

Estimated Log BCF = 0.500 (BCF = 3.162)

Reliability: (2) valid with restrictions
Accepted calculation method
27-JUN-2001 (1)

3.8 Additional Remarks

Remark: Degradation in natural water: 32-73 %
Source: Bayer AG Leverkusen
22-OCT-2001 (9)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: >= 100
Method: other: Letale Wirkung beim Zebrabaerbling, UBA-Verfahrensvorschlag, Mai 1984, Letale Wirkung beim Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h
Year: 1982 GLP: no
Test substance:
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
16-OCT-2001 (8)

Type:
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50: > 500
Method: other: Japanese Industrial Standard (JIS K 0102-1986-71) "Testing methods for industrial waste water"
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
16-OCT-2001 (7)

4.2 Acute Toxicity to Aquatic Invertebrates
Remark: Since the mono phosphate is expected to be more toxic than the tris-ester, the acute *Daphnia* LC_{50} of the tris-ester is expected to be greater than or equal to that of the bis-ester. Data for the mono- and bis-(2-ethyl hexyl) esters demonstrate 48 hr Acute Invertebrate LC_{50} to be >42 mg/l. (See IUCLID data sets on CAS#12645-31-7 and 298-07-7)

4.3 Toxicity to Aquatic Plants e.g. Algae
Remark: Acute toxicity to algae has been tested for 2-ethyl hexyl phosphate (12645-31-7) and demonstrated an EC_{50} of 161-168 mg/l (Table 3). Since the mono phosphate is expected to be more toxic than the tris-ester, the EC_{50} of the tris-ester is expected to be greater than or equal to 161 mg/l. (See IUCLID data set on CAS#12645-31-7)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: > 100
Method: other: see remarks
Chemosphere 10 (3), 245-261 (1981)
Year: 1982 GLP: no
Test substance:
Remark: direct weight
Method: E 3002: The Assessment of the Possible Inhibitory Effect of Dyestuffs on Aerobic Waste Water Bacteria. Experience with a Screening Test. Brown, D.; Hitz, H.R.; Schaefer, L.: Chemosphere 10 (3), 245-261 (1981)
Source: Bayer AG Leverkusen
28-JAN-1994 (8)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: 46000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
Flag: Critical study for SIDS endpoint
16-OCT-2001 (10)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 36800 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
Flag: Critical study for SIDS endpoint
16-OCT-2001 (11)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: ca. 46000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
16-OCT-2001 (11)

Type: LD0
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 10000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
Flag: Critical study for SIDS endpoint
16-OCT-2001 (12)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: 37080 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
Flag: Critical study for SIDS endpoint
16-OCT-2001 (13)

5.1.2 Acute Inhalation Toxicity

Type: other: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time: 4 hour(s)
Value: > .447 mg/l
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
16-OCT-2001 (11)

Type: other: LD50
Species: guinea pig
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time: 1 hour(s)
Value: > .46 mg/l
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
16-OCT-2001 (11)

Type: other: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value: > .45 mg/l
Method:
Year: GLP:
Test substance:
Remark: Exposure time: no data
Source: Bayer AG Leverkusen
16-OCT-2001 (10)

Type: other: LD50
Species: guinea pig
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value: 450 mg/l
Method:
Year: GLP:
Test substance:
Remark: Exposure time: no data
Source: Bayer AG Leverkusen
16-OCT-2001 (10)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: ca. 20000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
23-JUL-1992 (10)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.v.
Value: > 358 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
23-JUL-1992 (11)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: other: intratracheal
Value: > 1811 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
12-AUG-1992 (11)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other: see remarks
Year: GLP:
Test substance:
Remark: ear, 24 h exposure, dose not known
Source: Bayer AG Leverkusen
12-AUG-1992 (12)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other: see remarks
Year: GLP:
Test substance:
Remark: 250 mg applied to clipped skin on rabbit back, within 24 h moderate erythema which persisted for a week.
Source: Bayer AG Leverkusen
12-AUG-1992 (11)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: see remarks
Year: GLP:
Test substance:
Remark: 24 h exposure time
Source: Bayer AG Leverkusen
12-AUG-1992 (12)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method: other: see remarks
Year: GLP:
Test substance:
Remark: 0.01 to 0.5 ml, up to 0.05 ml slight conjunctivitits, from 0.1 to 0.5 ml moderate conjunctivities, which cleared up within 24 h
Source: Bayer AG Leverkusen
26-NOV-1992 (11)

5.3 Sensitization
-

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: other: F33/N
Route of admin.: gavage
Exposure period: 13 weeks
Frequency of treatment: 5 d/w
Post. obs. period: no
Doses: 250, 500, 1000, 2000 or 4000 mg/kg bw
Control Group: other: yes (corn oil)
NOAEL: 1000 mg/kg bw
LOAEL: 2000 mg/kg bw
Method: other: EPA OTS 798.3300
Year: GLP: yes
Test substance: other TS: tris(2-ethylhexyl) phosphate; purity 97-99%
Result: no compound related deaths, slight-moderate depression of weight gain at 2000 or 4000 mg/kg bw, no histopathologic effects.
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
17-OCT-2001 (14)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 13 weeks
Frequency of treatment: 5d/w
Post. obs. period: no
Doses: 500, 1000, 2000, 4000 or 8000 mg/kg bw/d
Control Group: other: yes (corn oil)
NOAEL: 2000 mg/kg bw
LOAEL: 4000 mg/kg bw
Method: other: EPA OTS 798.3300
Year: GLP: yes
Test substance: other TS: tris(2-ethylhexyl) phosphate; purity 97-99%
Result: No compound related deaths, slight-moderate depression of weight gain at 4000 or 8000 mg/kg bw, inflammatory lesions in gastric mucosa
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
22-OCT-2001 (14)

Species: rat Sex: no data
Strain: no data
Route of admin.: oral feed
Exposure period: 30 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 110 to 1550 mg/kg bw/d
Control Group: no data specified
NOAEL: 430 mg/kg
Method:
Year: GLP:
Test substance:
Result: at 1550 mg/kg weight loss
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
17-OCT-2001 (13)

Species: guinea pig Sex: male
Strain: Hartley
Route of admin.: inhalation
Exposure period: 3 months
Frequency of treatment: 6h/d, 5d/w
Post. obs. period: no
Doses: 1.6 and 9.6 mg/m3
Control Group: yes
NOAEL: 1.6 mg/m^3
LOAEL: 9.6 mg/m^3
Method:
Year: GLP:
Test substance: other TS: purity of substance not known
Result: at high level significantly increased terminal body weight, no significant alteration in red blood cell and plasma cholinesterase activity, no abnormalties at necropsy, microscopic examination revealed inconsistent and reversible changes of renal parenchyma of the high level group, sections of the spinal cord and sciatic nerve stained to demonstrate the myelin sheaths showed no pathologic alteration.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
16-OCT-2001 (11)

Species: dog Sex: male/female
Strain: other: mongrel dogs
Route of admin.: inhalation
Exposure period: 3 months
Frequency of treatment: 6h/d, 5d/w
Post. obs. period: no
Doses: 10.8, 26.4 or 85 mg/m3
Control Group: other: yes
Method:
Year: GLP:
Test substance:
Remark: purity unknown
Result: no deaths; evaluation of trained behavior: dose-response relationship in the conditioned avoidance response; no alterations in any of the hematological and biochemical parameters, normal increase in body weights, mild chronic inflammatory changes in pulmonary parenchyma.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
16-OCT-2001 (11)

Species: monkey Sex: male/female
Strain: other: Rhesus
Route of admin.: inhalation
Exposure period: 3 months
Frequency of treatment: 6h/d, 5d/w
Post. obs. period: no
Doses: 10.8, 26.4 or 85 mg/m3
Control Group: other: yes
NOAEL: 85
Method:
Year: GLP:
Test substance: other TS: purity of substance not known
Result: no deaths, normal weight gain, no alteration of any of the hematological and biochemical parameters, in the evaluation of trained behavior (visual discrimination test) no effects were detected. No histological abnormalities.
Source: Bayer AG Leverkusen
16-OCT-2001 (11)

Species: guinea pig Sex: male/female
Strain: Hartley
Route of admin.: inhalation
Exposure period: 3 months
Frequency of treatment: 6h/d, 5d/w, total 60 exposures
Post. obs. period: no
Doses: 10.8; 26.4 or 85 mg/m3
Control Group: yes
Method:
Year: GLP:
Test substance:
Result: high mortality in control group and dosed groups because of intercurrent respiratory infection.
Source: Bayer AG Leverkusen
16-OCT-2001 (11)

Species: rabbit Sex: no data
Strain: other: New Zealand
Route of admin.: dermal
Exposure period: 2 to 4 weeks
Frequency of treatment: 5 d/w
Post. obs. period: 3 - 17 d
Doses: 0.1 ml/animal
Control Group: no
Method:
Year: GLP:
Test substance:
Result: animals appeared normal and gained weight, no alterations were observed at necropsy. Skin: moderate erythema following the first application, following subsequent applications, the erythema did not increase in intensity, but a gradual increase in the size of the affected zone was observed. After the fifth application desquamination, hemorrhagic areas, thickening of the skin. Microscopic examination: hyperkeratosis, parakeratosis, good recovery.
Source: Bayer AG Leverkusen
16-OCT-2001 (11)

Species: rat Sex: male/female
Strain: other: F344/N
Route of admin.: gavage
Exposure period: 14 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 375, 750, 1500, 3000 or 6000
Control Group: other: yes (corn oil)
Method:
Year: GLP:
Test substance:
Result: No animals died, reduced weight gain in male at 1500 mg/kg and higher, in female at 3000 or 6000 mg/kg. No compound related effects at necropsy
Source: Bayer AG Leverkusen
22-OCT-2001 (14)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 14 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 375, 750, 1500, 3000 or 6000 mg/kg bw/d
Control Group: other: yes (corn oil)
Method:
Year: GLP:
Test substance:
Result: No animals died. No changes in body weight gain, no compound-related effects at necropsy
Source: Bayer AG Leverkusen
17-OCT-2001 (14)

Species: cat Sex: no data
Strain: no data
Route of admin.: gavage
Exposure period: 28 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 1 ccm/kg bw/d
Control Group: no
Method:
Year: GLP:
Test substance:
Result: no clinical signs of toxicity, no inhibition of cholinesterase activity in red blood cells.
Source: Bayer AG Leverkusen
16-OCT-2001 (12)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: S. typhimurium TA 98, 100, 1535, 1537
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
16-OCT-2001 (14)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration:
Cytotoxic Conc.:
Metabolic activation: no data
Result: negative
Method:
Year: GLP:
Test substance:
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
16-OCT-2001 (15) (16) (17) (18)

Type: other: Chromosomal aberration
System of testing: CHO-cells
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Flag: Critical study for SIDS endpoint
16-OCT-2001 (15) (16) (19) (18)

Type: Sister chromatid exchange assay
System of testing: CHO-cells
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Flag: Critical study for SIDS endpoint
16-OCT-2001 (15) (16) (19) (18)

Type: Ames test
System of testing: S. typhimurium TA98, 100, 1535, 1537
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
23-JUL-1992 (20)

Type: Ames test
System of testing: S. typhimurium
Concentration:
Cytotoxic Conc.:
Metabolic activation: no data
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
23-JUL-1992 (15) (16) (18)

Type: Ames test
System of testing: S. typhimurium TA 98, TA100, TA1535, TA 1537
Concentration:
Cytotoxic Conc.:
Metabolic activation: with
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
23-JUL-1992 (21)

Type: Ames test
System of testing: S. typhimurium TA98, TA100, TA1535, TA1537
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Remark: purity 97.6 %
Source: Bayer AG Leverkusen

23-JUL-1992 (22)

5.6 Genetic Toxicity 'in Vivo'
-

5.7 Carcinogenicity

Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 2 years
Frequency of treatment: 5 d/w
Post. obs. period: no
Doses: male 2000 or 4000 mg/kg bw/d, female 1000 or 2000 mg/kg bw/d
Result:
Control Group: other: yes (corn oil)
Method: EPA OTS 798.3300
Year: GLP: yes
Test substance: other TS: tris(2-ethylhexyl)phosphate; Purity 97-98 %
Result: no clinical signs of toxicity, depression in body weights only in male animals, survival unaffected, incidence of pheochromocytoma of adrenal glands increased with dose, positive trend for increased incidence of thyroid follicular cell hyperplasia in male rats. In female rats no evidence of carcinogenicity, in male rats equivocal evidence of carcinogenicity in the adrenal gland medulla
Reliability: (1) valid without restriction
GLP Guideline study

17-OCT-2001 (23) (24) (25) (14)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 2 years
Frequency of treatment: 5d/w
Post. obs. period: no
Doses: 500 or 1000 mg/kg bw
Result:
Control Group: other: yes (corn oil)
Method: EPA OTS 798.3300
Year: GLP: yes
Test substance: other TS: tris(2-ethylhexyl)phosphate; Purity 97-98 %
Result: no clinical signs of toxicity, no depression in body weights, survival unaffected, increased incidence of follicular cell hyperplasias of the thyroid gland in males and females. No evidence of carcinogenicity in male mice, some evidence of carcinogenicity in female mice (hepatocellular carcinoma).
Reliability: (1) valid without restriction

GLP Guideline study

17-OCT-2001 (23) (24) (25) (14)

Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 24 months
Frequency of treatment: 5 days/week
Post. obs. period: none
Doses: 50, 150, 500 mg/kg/day
Result: negative
Control Group: yes, concurrent vehicle
Method: EPA OTS 798.3300
Year: GLP: yes
Test substance: other TS: 2-ETHYLHEXANOL; purity > 99%
Remark: 2-ethylhexanol is used in the preparation of tris(2-ethylhexyl)phosphate and believed to be the major metabolic product.
Result: In decedent and surviving male and female rats recieving 2EH, the incidence of basophilic, eosinophilic, and clear cell foci and focal hyperplasia was not different from that in the vehicle controls. There was no increase in the incidence of hepatocellular carcinomas in rats treated with 2EH.
Reliability: (1) valid without restriction

GLP Guideline study

17-OCT-2001 (26)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 18 months
Frequency of treatment: 5 days/week
Post. obs. period: none
Doses: 50, 200, 750 mg/kg/day
Result:
Control Group: yes, concurrent vehicle
Method: EPA OTS 798.3300
Year: GLP: yes
Test substance: other TS: 2-ETHYLHEXANOL; purity > 99%
Remark: 2-ethylhexanol is used in the preparation of tris(2-ethylhexyl)phosphate and believed to be the major metabolic product.
Result: In surviving female mice, there were no eosinophilic foci and no adenomas and a single hyperplastic focus at 200 mg/kg. There appears to be a correlation between the increased incidence of basophilic foci and hepatocellular carcinomas in female mice, however the increases were only significant at 750 mg/kg.
The preneoplastic changes in the livers of female mice, while suggestive of weak oncogenicity, are not conclusive.
Reliability: (1) valid without restriction

GLP Guideline study
17-OCT-2001 (26)

5.8 Toxicity to Reproduction

Remark: Adequate reproductive and developmental studies are available for the two similar chemicals (107-66-4 and 126-73-8). These studies indicate an absence of reproductive or developmental effects of these chemicals at doses ranging from >225 to 1000 mg/kg. Since repeat dose testing of this category demonstrates an apparent reduction in toxicity with increasing molecular weight, no reproductive or developmental effects of tris (2-ethyl hexyl) phosphate (78-42-2) is expected at doses ranging from >225 to 1000 mg/kg. (See IUCLID data sets on CAS#107-66-4 and 126-73-8)

5.9 Developmental Toxicity/Teratogenicity

Remark: Adequate reproductive and developmental studies are available for the two similar chemicals (107-66-4 and 126-73-8). These studies indicate an absence of reproductive or developmental effects of these chemicals at doses ranging from >225 to 1000 mg/kg. Since repeat dose testing of this category demonstrates an apparent reduction in toxicity with increasing molecular weight, no reproductive or developmental effects of tris (2-ethyl hexyl) phosphate (78-42-2) is expected at doses ranging from >225 to 1000 mg/kg. (See IUCLID data sets on CAS#107-66-4 and 126-73-8)
and 126-73-8)

5.10 Other Relevant Information

Type:
Remark: hen, gavage: 250, 500 or 1000 mg/kg bw, single application: post exposure examination 2 months, no clinical signs of neurotoxicity.
hen: i.m.: 250, 500 or 1000 mg/kg bw: no clinical signs of toxicity.
Source: Bayer AG Leverkusen
03-JUN-1993 (12)

Type:
Remark: human cells, in vitro: HeLa-Cells, Metabolic Inhibition Test, 24 h inkubation: no acute toxicity
Source: Bayer AG Leverkusen
23-JUL-1992 (27)

Type:
Remark: hen, single oral dose, 500 or 2500 mg/kg bw, 1 high level animal died, the other appeared normal and maintained or gained weight; macroscopic examination revealed no abnormalities, histological no evidence of demyelinizing action.
Source: Bayer AG Leverkusen
23-JUL-1992 (11)

Type:
Remark: Radiotracer inhalation study with rats: 9 male rats, single head exposure, 20 minutes, aerosol, sacrifice after 5 min, 30 min, 1, 4, 17, 18, 24, 48, or 70 h:analytcal concentration 0.72 to 0.91 mg/l, maximum retention in tissue after the first few hours, fecal excretion high.
Source: Bayer AG Leverkusen
23-JUL-1992 (11)

Type:
Method: The "Total Diet Study" uses dietary survey information and analysis of individual food items, and assessed daily intakes of a number of age-sex groups.
Remark: The mean daily intake per unit of body weight

age:	(ug/kg bw/day)
6-11 months	0.0015
2 year	0.0051
14-16 (female)	0.0029
14-16 (male)	0.0033
25-30 (female)	0.0039
25-30 (male)	0.0055
60-65 (female)	0.0033
60-65 (male)	0.0037

16-OCT-2001 (28)

5.11 Experience with Human Exposure
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7.1 End Point Summary

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7.2 Hazard Summary

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7.3 Risk Assessment

-

201-16174B

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IUCLID

Data Set

Existing Chemical	:	ID: 7664-38-2
CAS No.	:	7664-38-2
EINECS Name	:	orthophosphoric acid
EC No.	:	231-633-2
TSCA Name	:	Phosphoric acid
Molecular Formula	:	H3O4P

Producer related part

Company	:	EUROPEAN COMMISSION - European Chemicals Bureau
Creation date	:	11.02.2000

Substance related part

Company	:	EUROPEAN COMMISSION - European Chemicals Bureau
Creation date	:	11.02.2000
Status	:	
Memo	:	
Printing date	:	24.08.2004
Revision date	:	11.02.2000
Date of last update	:	11.02.2000
Number of pages	:	75
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

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Homepage	:	

Type	:	
Name	:	Leduc Chemie B.V.
Contact person	:	
Date	:	
Street	:	Printerweg 17
Town	:	3821 AP Amersfoort
Country	:	Netherlands
Phone	:	(31) 33-4561006
Telefax	:	(31) 33-4562692
Telex	:	43501 leduc
Cedex	:	unknown
Email	:	
Homepage	:	

Type	:	
Name	:	MB SVEDA AB
Contact person	:	
Date	:	
Street	:	Box 4072
Town	:	203 11 Malmö
Country	:	Sweden
Phone	:	0094640352800
Telefax	:	0094640125172
Telex	:	33188
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	NEUBER GES.M.B.H.
Contact person	:	
Date	:	
Street	:	BRÜCKENGASSE 1
Town	:	1060 WIEN
Country	:	Austria
Phone	:	0222/599950
Telefax	:	0222/5970200
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Penta Chemikalien GmbH
Contact person	:	
Date	:	
Street	:	Hanauer Straße 70 - 74
Town	:	63739 Aschaffenburg
Country	:	Germany
Phone	:	06021/21201 + 15873
Telefax	:	06021/21206

Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Prayon-Rupel S.A.
Contact person	:	
Date	:	
Street	:	Rue Joseph Wauters 144
Town	:	4480 Engis
Country	:	Belgium
Phone	:	32 41 73 92 83
Telefax	:	32 41 75 01 68
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Quimigal Adubos SA.
Contact person	:	
Date	:	
Street	:	Av. Infante Santo, nº 2 - 2º
Town	:	1100 Lisboa
Country	:	Portugal
Phone	:	3979161
Telefax	:	3977716
Telex	:	12426
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Rhone-Poulenc Chemie N.V.
Contact person	:	
Date	:	
Street	:	
Town	:	9020 Gent
Country	:	Belgium
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Rhone-Poulenc Chimie
Contact person	:	
Date	:	
Street	:	25, Quai Paul Doumer
Town	:	92408 Courbevoie Cedex
Country	:	France
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Email	:	
Homepage	:	

Type	:	
Name	:	Rhone-Poulenc Quimica SA
Contact person	:	
Date	:	
Street	:	
Town	:	21001 Huelva
Country	:	Spain
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Riedel-de Haën AG
Contact person	:	
Date	:	
Street	:	Wunstorfer Str.40
Town	:	30926 Seelze
Country	:	Germany
Phone	:	05137 999 0
Telefax	:	05137 999 123
Telex	:	9 21 295 rdhs d
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	ROTEM FERTILIZERS LTd
Contact person	:	
Date	:	
Street	:	HAORGIM
Town	:	77051 ASHDOD
Country	:	other: Israel
Phone	:	9728511520
Telefax	:	9728560219
Telex	:	381890 PHOS IL
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	S.A.I. Societa' Approvv. Indutriali Spa
Contact person	:	
Date	:	
Street	:	Tulipani n. 1
Town	:	20090 Pieve Emanuele (MI)
Country	:	Italy
Phone	:	+39/015/2546711
Telefax	:	+39/015/2546750
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Schering AG
Contact person	:	
Date	:	
Street	:	
Town	:	13587 Berlin
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Shell Nederland Chemie B.V.
Contact person	:	
Date	:	
Street	:	Vondelingenweg 601
Town	:	3196 KK Rotterdam
Country	:	Netherlands
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	SIRIAC
Contact person	:	
Date	:	
Street	:	C.DA PEZZA DI RIZZO
Town	:	97011 ACATE
Country	:	Italy
Phone	:	0932 989880
Telefax	:	0932 989383
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	Stickstoffwerke AG
Contact person	:	
Date	:	
Street	:	Dessauer Str. 126
Town	:	06886 Lu. Wittenberg
Country	:	Germany
Phone	:	03491/684001
Telefax	:	03491/684569
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	ThermPhos International B.V.
Contact person	:	
Date	:	
Street	:	P.O. Box 406
Town	:	4380 AK Vlissingen
Country	:	Netherlands
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	VOLKERS BENELUX B.V.
Contact person	:	
Date	:	
Street	:	INDUSTRIEWEG 1
Town	:	1230 AC LOOSDRECHT
Country	:	Netherlands
Phone	:	+31 35 588 92 00
Telefax	:	+31 35 582 43 64
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	VOS B.V.
Contact person	:	
Date	:	
Street	:	Ondernemingsweg 1A
Town	:	2404 HM Alphen aan den Rijn
Country	:	Netherlands
Phone	:	31-172-431601
Telefax	:	31-172-432494
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Type	:	
Name	:	ZENECA Specialties
Contact person	:	
Date	:	
Street	:	PO Box 42
Town	:	M9 3DA Manchester
Country	:	United Kingdom
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : inorganic
Physical status : liquid
Purity : -
Colour :
Odour :

Purity type :
Substance type : inorganic
Physical status : solid
Purity : -
Colour :
Odour :

Purity type :
Substance type : inorganic
Physical status :
Purity : -
Colour :
Odour :

Purity type :
Substance type : organic
Physical status : liquid
Purity : -
Colour :
Odour :

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

3M Etching Liquid

Source : Henkel KGaA Duesseldorf

Acide orthophosphorique

Source : CECA SA Paris-La Defence 2

ACIDE PHOSPHORIQUE DE VOIE HUMIDE

Source : Prayon-Rupel S.A. Engis

Acido fosforico...%

Source : S.A.I. Societa" Approvv. Indutriali Spa Pieve Emanuele (MI)

Acido fosfórico

Source : FMC FORET SA BARCELONA

ACIDO ORTOFOSFORICO

Source : SIRIAC ACATE

Acido ortofosfórico

Source : FMC FORET SA BARCELONA

acidum phosphoricum

Source : Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Henkel KGaA Duesseldorf

acidum phosphoricum (INN)

Source : Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Henkel KGaA Duesseldorf

C 134

Source : Henkel KGaA Duesseldorf

C 134 (acid)

Source : Henkel KGaA Duesseldorf

C 434

Source : Henkel KGaA Duesseldorf

C 434 (acid)

Source : Henkel KGaA Duesseldorf

Decon 4512

Source : Henkel KGaA Duesseldorf

E 338

Source : Henkel KGaA Duesseldorf

EVITs

Source : Henkel KGaA Duesseldorf

H3PO4

Source : Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Henkel KGaA Duesseldorf

Hydrogen phosphate

Source : ELF ATOCHEM Paris la defense 10

K-etchant

Source : Henkel KGaA Duesseldorf

Kefo

Source : Henkel KGaA Duesseldorf

Mikro Klene DF

Source : Henkel KGaA Duesseldorf

ortho - Phosphorsäure

Source : Riedel-de Haën AG Seelze

ortho-Phosphorsaeure

Source : Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Hoechst AG Frankfurt/Main
Henkel KGaA Duesseldorf

ortho-Phosphorsäure

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Krems Chemie AG Krems

Ortho-Phosphorsäure

Source : Penta Chemikalien GmbH Aschaffenburg

Orthofosforzuur

Source : VOS B.V. Alphen aan den Rijn

Orthophosphoric acid

Source : Hydro Agri Rotterdam B.V Vlardingen
Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
BASF AG Ludwigshafen
BASF Antwerpen N. V. Antwerpen 4
ELF ATOCHEM Paris la defense 10
Hydro Agri France S.A. Neuilly-Sur-Seine
Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Henkel KGaA Duesseldorf

orthophosphoric acid

Source : Kemira Ince Ltd Ince, Chester

Orthophosphoric Acid

Source : Henkel KGaA Duesseldorf

ORTHOPHOSPHORIC ACID

Source : ROTEM FERTILIZERS LTd ASHDOD

Orthophosphoric acid.

Source : "Hawley's Condensed Chemical Dictionary"; revised by N.Irving Sax and Richard J. Lewis,Sr.; eleventh edition; 1985; New York: Van Nostrand Reinhold; p.910.
Leduc Chemie B.V. Amersfoort

Orthophosphorsaure

Source : CECA SA Paris-La Defence 2

Orthophosphorsäure

Source : Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
NEUBER GES.M.B.H. WIEN
Henkel KGaA Duesseldorf

P-0620 T 1/8"

Source : Henkel KGaA Duesseldorf

phosphoric acid

Source : Shell Nederland Chemie B.V. Rotterdam
Kemira Ince Ltd Ince, Chester

Phosphoric acid

Source : Rhone-Poulenc Chemie N.V. Gent
ELF ATOCHEM Paris la defense 10
CECA SA Paris-La Defence 2
Rhone-Poulenc Quimica SA Huelva
Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Albright & Wilson Ltd. Warley
Albright & Wilson Oldbury, Warley, West Midlands
Henkel KGaA Duesseldorf

PHOSPHORIC ACID

Source : Enichem Agricoltura Milan
ROTEM FERTILIZERS LTd ASHDOD

Phosphoric Acid

Source : HI-AGRI SRL Bologna

Phosphoric acid (7Cl, 8Cl, 9Cl)

Source : BASF AG Ludwigshafen
BASF Antwerpen N. V. Antwerpen 4

Phosphoric acid (7CI, 8CI, 9CI) (CA INDEX NAME)

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Henkel KGaA Duesseldorf

Phosphoric acid (INCI)

Source : Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Henkel KGaA Duesseldorf

Phosphoric acid (INCI) (INN)

Source : Henkel KGaA Duesseldorf

phosphoric acid (INN)

Source : Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Henkel KGaA Duesseldorf

Phosphoric acid, Fosforihappo

Source : Kemira Chemicals OY Helsinki

PHOSPHORIC ACID, ortho; PHOSPHORIC ACID;PHOSACID;WET PROCESS PHOSACID

Source : Grande Paroisse SA Paris la Defense 5

Phosphoric acid, Orthophosphoric acid

Source : Amsterdam Fertilers b.v Amsterdam

Phosphorsaeure

Source : BASF AG Ludwigshafen
BASF Antwerpen N. V. Antwerpen 4
Henkel Austria Ges.m.b.H.
Henkel Austria Ges.m.b.H. Wien
Hoechst AG Frankfurt/Main
Henkel KGaA Duesseldorf

Phosphorsäure

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Krems Chemie AG Krems
Henkel KGaA Duesseldorf
Schering AG Berlin
Penta Chemikalien GmbH Aschaffenburg

Sonac

Source : Henkel KGaA Duesseldorf

Thermische Phosphorsaeure

Source : Hoechst AG Frankfurt/Main
Henkel KGaA Duesseldorf

Thermische Phosphorsäure

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Henkel KGaA Duesseldorf

WC-Reiniger

Source : Henkel KGaA Duesseldorf

wet process phosphoric acid

Source : Kemira Ince Ltd Ince, Chester

WHITE PHOSPHORIC ACID

Source : ROTEM FERTILIZERS LTd ASHDOD

ácido fosfórico

Source : Quimigal Adubos SA. Lisboa

Source : Prayon-Rupel S.A. Engis

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

Quantity : > 1000000 - tonnes in

1.6.1 LABELLING

Labelling : as in Directive 67/548/EEC
Specific limits : yes
Symbols : C, , ,
Nota : B, E,
R-Phrases : (34) Causes burns
S-Phrases : (1/2) Keep locked up and out of reach of children
(26) In case of contact with eyes, rinse immediately with plenty of water and seek medical advice
(45) In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible)

1.6.2 CLASSIFICATION

Classified	:	as in Directive 67/548/EEC
Class of danger	:	corrosive
R-Phrases	:	(34) Causes burns
Specific limits	:	

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	type
Category	:	Non dispersive use

Type of use	:	type
Category	:	Use in closed system

Type of use	:	type
Category	:	Wide dispersive use

Type of use	:	industrial
Category	:	Agricultural industry

Type of use	:	industrial
Category	:	Basic industry: basic chemicals

Type of use	:	industrial
Category	:	Chemical industry: used in synthesis

Type of use	:	industrial
Category	:	Electrical/electronic engineering industry

Type of use	:	industrial
Category	:	Leather processing industry

Type of use	:	industrial
Category	:	Metal extraction, refining and processing of metals

Type of use	:	industrial
Category	:	Paints, lacquers and varnishes industry

Type of use	:	industrial
Category	:	Personal and domestic use

Type of use	:	industrial
Category	:	Polymers industry

Type of use : industrial
Category : Public domain

Type of use : industrial
Category : Textile processing industry

Type of use : industrial
Category : other: Food Industry

Type of use : industrial
Category : other: Industrial

Type of use : industrial
Category : other: FOOD INDUSTRY

Type of use : industrial
Category : other: LIQUID CLEANERS

Type of use : industrial
Category : other: METAL TREATMENT

Type of use : industrial
Category : other: fertilizer production

Type of use : industrial
Category : other

Type of use : use
Category : Cleaning/washing agents and disinfectants

Type of use : use
Category : Complexing agents

Type of use : use
Category : Conductive agents

Type of use : use
Category : Corrosive inhibitors

Type of use : use
Category : Electroplating agents

Type of use : use
Category : Fertilizers

Type of use : use

Category	:	Food/foodstuff additives
Type of use	:	use
Category	:	Intermediates
Type of use	:	use
Category	:	Laboratory chemicals
Type of use	:	use
Category	:	pH-regulating agents
Type of use	:	use
Category	:	Process regulators
Type of use	:	use
Category	:	Solvents
Type of use	:	use
Category	:	Stabilizers
Type of use	:	use
Category	:	Surface-active agents
Type of use	:	use
Category	:	Tanning agents
Type of use	:	use
Category	:	Welding and soldering agents
Type of use	:	use
Category	:	other: treat drinking water
Type of use	:	use
Category	:	other: Product in many use applications.
Type of use	:	use
Category	:	other: cf remarque
Type of use	:	use
Category	:	other: see RM
Type of use	:	use
Category	:	
Type of use	:	use
Category	:	other

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : MAC (NL)
Limit value : 1 mg/m3

Source : Hydro Agri Rotterdam B.V Vlardingen
Based on specifications for UN-number 1805.
Leduc Chemie B.V. Amersfoort
Hydro Agri France S.A. Neuilly-Sur-Seine

Type of limit : MAC (NL)
Limit value : 1 mg/m3
Short term exposure limit value
Limit value : 2 mg/m3
Time schedule : 15 minute(s)
Frequency : times

Source : VOLKERS BENELUX B.V. LOOSDRECHT

Type of limit : MAK (DE)
Limit value :

Remark : Kein MAK-Wert festgelegt
Source : BASF AG Ludwigshafen
BASF Antwerpen N. V. Antwerpen 4

(1)

Type of limit : MAK (DE)
Limit value :

Source : Stickstoffwerke AG Lu. Wittenberg

Type of limit : MAK (DE)
Limit value : 1 mg/m3

Source : ROTEM FERTILIZERS LTd ASHDOD

Type of limit : OES (UK)
Limit value : 1 mg/m3
Short term exposure limit value
Limit value : 3 mg/m3
Time schedule :
Frequency : times

Source : Hydro Agri Rotterdam B.V Vlardingen
Hydro Agri France S.A. Neuilly-Sur-Seine

Type of limit : OES (UK)

Limit value : 1 mg/m3
Short term exposure limit value
Limit value : 3 mg/m3
Time schedule : 10 minute(s)
Frequency : times

Source : Albright & Wilson Ltd. Warley
Kemira Ince Ltd Ince, Chester
Albright & Wilson Oldbury, Warley, West Midlands

Type of limit : TLV (US)
Limit value : 1 mg/m3
Short term exposure limit value
Limit value : 3 mg/m3
Time schedule :
Frequency : times

Source : Amsterdam Fertilers b.v Amsterdam
Prayon-Rupel S.A. Engis
Exposure limits for orthophosphorique acid : US-ACGIH 1995.
ELF ATOCHEM Paris la defense 10
Quimigal Adubos SA. Lisboa
Enichem Agricoltura Milan

Type of limit : TLV (US)
Limit value : 1 mg/m3

Source : BASF AG Ludwigshafen
BASF Antwerpen N. V. Antwerpen 4

(2)

Type of limit : TLV (US)
Limit value : 1 mg/m3
Short term exposure limit value
Limit value : 3 mg/m3
Time schedule : 15 minute(s)
Frequency : times

Source : Rhone-Poulenc Chemie N.V. Gent
Rhone-Poulenc Chimie Courbevoie Cedex
Rhone-Poulenc Quimica SA Huelva

Type of limit : TLV (US)
Limit value : 1 mg/m3
Short term exposure limit value
Limit value : 3 mg/m3
Time schedule :
Frequency : times

Remark : ACGIH TLV review; TWA 1mg/m3; STEL 3 mg/m3
NIOSH Recommended Limits NREC; NIOSH REL to Phosphoric acid-air 10h TWA 1 mg/m3; STEL 3 mg/m3
OSHA PEL FINAL 8H TWA 1mg/m3; STEL 3 mg/m3
OEL Australia, Belgium, Denmark, Egypt, Finland, France, Japan, Netherlands, Philippines, Switzerland, Thailand, UK: TWA 1mg/m3; Australia, Belgium, Finland, France, Sweden, UK:STEL 3mg/m3.
Source : Grande Paroisse SA Paris la Defense 5

(3)

Type of limit : TLV (US)
Limit value : 1 mg/m3

Short term exposure limit value
Limit value : 3 mg/m3
Time schedule : 60 minute(s)
Frequency : 1 times

Source : S.A.I. Societa" Approvv. Indutriali Spa Pieve Emanuele (MI)

Type of limit : other: HTP (FIN)
Limit value : 1 mg/m3
Short term exposure limit value
Limit value : 3 mg/m3
Time schedule : 15 minute(s)
Frequency : times

Source : Kemira Chemicals OY Helsinki

Type of limit : other: MAC-TGG
Limit value : 1.2 mg/m3
Short term exposure limit value
Limit value : 2 mg/m3
Time schedule :
Frequency : times

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(4)

Type of limit : other: VME(FR)
Limit value : 1 mg/m3
Short term exposure limit value
Limit value : 3 mg/m3
Time schedule : 15 minute(s)
Frequency : times

Source : Rhone-Poulenc Chemie N.V. Gent
Rhone-Poulenc Chimie Courbevoie Cedex
Rhone-Poulenc Quimica SA Huelva

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

Classified by : KBwS (DE)
Labelled by : KBwS (DE)
Class of danger : 1 (weakly water polluting)

Remark : Kenn-Nr. 392
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(5) (6)

Classified by : KBwS (DE)
Labelled by : KBwS (DE)
Class of danger : 1 (weakly water polluting)

Source : BASF AG Ludwigshafen
BASF Antwerpen N. V. Antwerpen 4

Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	1 (weakly water polluting)
Source	:	BASF AG Ludwigshafen BASF Antwerpen N. V. Antwerpen 4
Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	1 (weakly water polluting)
Source	:	BASF AG Ludwigshafen BASF Antwerpen N. V. Antwerpen 4
Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	1 (weakly water polluting)
Source	:	BASF AG Ludwigshafen BASF Antwerpen N. V. Antwerpen 4
Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	1 (weakly water polluting)
Source	:	BASF AG Ludwigshafen
Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	1 (weakly water polluting)
Source	:	BASF AG Ludwigshafen
Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	1 (weakly water polluting)
Remark	:	Kenn-Nr. 392
Source	:	Hoechst AG Frankfurt/Main

(5) (7)

1.8.4 MAJOR ACCIDENT HAZARDS

Legislation	:	Stoerfallverordnung (DE)
Substance listed	:	no
No. in Seveso directive	:	
Source	:	BASF AG Ludwigshafen BASF Antwerpen N. V. Antwerpen 4

(8)

Legislation	:	Stoerfallverordnung (DE)
Substance listed	:	no
No. in Seveso directive	:	
Source	:	Hoechst AG Frankfurt/Main

(7)

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark : We have no information about the production process or the number of producing facilities.
Source : Leduc Chemie B.V. Amersfoort

Remark : Fabrication par attaque d'un minerai de phosphate par H2 SO4, filtration, concentration et purification par extraction liquide liquide.

Effluent solide de gypse provenant de l'attaque.

Effluent aqueux legerement acide provenant de la purication.
Source : Rhone-Poulenc Chemie N.V. Gent

Country : BELGIQUE
Remark : UNITE DE PRODUCTION A ENGIS.
Source : Prayon-Rupel S.A. Engis

Remark : Fabrication par attaque d'un minerai de phosphate par H2 SO4, filtration, concentration et purification par extraction liquide liquide.

Effluent solide de gypse provenant de l'attaque.

Effluent aqueux legerement acide provenant de la purication.
Source : Rhone-Poulenc Chimie Courbevoie Cedex

Remark : Production process : Polyphosphoric acid is made by reactionbetween phosphoric acid and phosphorous oxide. One production plant.
Individual protective equipment (Gloves, goggles, protective chlothing, face-mask).
Source : ELF ATOCHEM Paris la defense 10

Remark : Fabrication par attaque d'un minerai de phosphate par H2 SO4, filtration, concentration et purification par extraction liquide liquide.

Effluent solide de gypse provenant de l'attaque.

Effluent aqueux legerement acide provenant de la purication.

Source : Rhone-Poulenc Quimica SA Huelva

Remark : Il prodotto viene acquistato sfuso e rivenduto tal quale. Sipossono verificare spandimenti accidentali di quantita' irrisorie di sostanza.

Source : S.A.I. Societa" Approvv. Indutriali Spa Pieve Emanuele (MI)

Remark : All information in section is CONFIDENTIAL.

Source : Albright & Wilson Ltd. Warley

Remark : Phosphoric acid brought into Ince is stored as a liquid in rubber-lined tanks before being pumped to Pipe Reactors for the production of ammonium phosphate for complex fertiliser manufacture (see submission for ammonium phosphate).

The resulting solid fertiliser is handled by industrial operators, merchants and farm workers.

Source : Kemira Ince Ltd Ince, Chester

Remark : All information in section is CONFIDENTIAL.

Source : Albright & Wilson Oldbury, Warley, West Midlands

Remark : Not available

Source : Kemira Chemicals OY Helsinki

Remark : 1.THE SUBSTANCE IS A RAW MATERIAL IN THE PRODUCTION OF FINAL PRODUCTS .POTENTIAL HUMAN OR ENVIRONMENTAL EXPOSURE COULD BE VIA THE FINAL PRODUCT LIFE CYCLE.

2.THE SUBSTANCE IS PRODUCED IN ISRAEL(NON EEC COUNTRY).

Source : ROTEM FERTILIZERS LTd ASHDOD

1.11 ADDITIONAL REMARKS

Source : Shell Nederland Chemie B.V. Rotterdam

Remark : This product has a 8, 17c RID/ADR/ADNR classification.

Source : Leduc Chemie B.V. Amersfoort

Remark : - Pollution de l'eau :
classification et etiquetage KBwS (DE)
categorie de danger WGK : 1

- Substance non listee dans la Directive SEVESO 82/501/CEE.¶

Source : Rhone-Poulenc Chemie N.V. Gent

Remark : - Pollution de l'eau :

classification et etiquetage KBwS (DE)
categorie de danger WGK : 1

- Substance non listee dans la Directive SEVESO 82/501/CEE.¶

Source : Rhone-Poulenc Chimie Courbevoie Cedex

Remark : Corrosive to ferrous metals and alloys
Source : Grande Paroisse SA Paris la Defense 5

Remark : Transport information :
UN number: 1805
ADR/RID: Class:8; Item (letter):17°c;
Prescriptions: Labels:8; H.I. Nr/ID Nr:80/1805;
IMDG : Class:8; Packaging group:III; UN Nr (IMDG):1805;
Prescriptions: Labels:8;
IATA : Class:8; Packaging group:III; UN Nr(IATA) or ID Nr:1805.
Prescriptions: Labels:8.

Source : ELF ATOCHEM Paris la defense 10

Remark : - Pollution de l'eau :
classification et etiquetage KBwS (DE)
categorie de danger WGK : 1

- Substance non listee dans la Directive SEVESO 82/501/CEE.¶

Source : Rhone-Poulenc Quimica SA Huelva

Remark : Not available
Source : Kemira Chemicals OY Helsinki

Remark : STORAGE

THE ACID STORAGE TANKS CAN BE MADE OF STAINLESS STEEL, RUBBERLINED STEEL OR VARRIOUS PLASTICS.
TRANSPORTATION REGULATIONS

PHOSPHORIC ACID IS LISTED AS UN NUMBER 1805.
RID/ADR: CLASS 8, 11C
IMDG: CLASS 8
IATA: CLASS 8 PACKAGING GROUP III
WATER POLLUTION

KBWS(DE) CLASS OF DANGER: 1 (WEEKLY WATER POLLUTING)

Source : ROTEM FERTILIZERS LTd ASHDOD

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : ca. -20 - 0 °C
Decomposition : no, at - °C
Sublimation : no
Method : other
Year :
GLP :
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
Test substance : melting point for aqueous solutions between 75 and 80% phosphoric acid as produced. Pure phosphoric acid solutions may differ due to absence of impurities ie.:
75% soln. - 17.5°C
80% soln. + 4.6°C
85% soln. + 21°C

Value : = -20 - °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphoräure 75 %ig

(9)

Value : = 3 - °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphorsäure 80 %ig

(9)

Value : = 21 - °C

Remark : Erstarrungspunkt
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphorsäure rein 85 %
Die Angaben zur Reinheit beziehen sich auf die Handelsware und nicht auf produzierte H3PO4.

(9) (6)

Value : = 21 - °C

Source : Hoechst AG Frankfurt/Main
Test substance : Phosphorsaeure 85 %ig

(10) (7)

Value : = 42.4 - °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphorsäure kristallin

(11)

Value : 42.4 - °C
Sublimation :
Method : other
Year : 1989

GLP	:	no
Test substance	:	
Source	:	Grande Paroisse SA Paris la Defense 5
Test substance	:	100% H3PO4, see ref (2)
Value	:	= 42.4 - °C
Source	:	Hoechst AG Frankfurt/Main
Test substance	:	Phosphorsaeure kristallin

(11)

Value	:	= - -17.5 °C
Decomposition	:	no, at - °C
Sublimation	:	no
Method	:	other
Year	:	1998
GLP	:	no data
Test substance	:	
Source	:	Based on a rapport from our Polish supplier (see paragraph 1.04). Leduc Chemie B.V. Amersfoort

2.2 BOILING POINT

Value	:	ca. 133 - °C at 1013 hPa
Decomposition	:	ambiguous
Method	:	
Year	:	
GLP	:	
Test substance	:	
Source	:	Grande Paroisse SA Paris la Defense 5
Test substance	:	75% aqueous solution of phosphoric acid
Value	:	= 135 - °C at 1013 hPa
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen
Test substance	:	Phosphoräure 75 %ig

(9)

Value	:	> 135 - °C at 1013 hPa
Decomposition	:	
Method	:	other
Year	:	1994
GLP	:	no data
Test substance	:	
Source	:	Grande Paroisse SA Paris la Defense 5

(12)

Value	:	> 135 - °C at
Source	:	BASF AG Ludwigshafen

(13)

Value	:	= 145 - °C at 1013 hPa

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphorsäure 80 %ig
(9)

Value : = 158 - °C at 1013 hPa

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphorsäure rein 85 %
Die Angaben zur Reinheit beziehen sich auf die Handelsware und nicht auf produzierte H3PO4.
(9) (6)

Value : = 158 - °C at 1013 hPa

Source : Hoechst AG Frankfurt/Main
Test substance : Phosphorsaeure 85 %ig
(10) (7)

Value : ca. 158 - °C at
Decomposition :
Method : other
Year :
GLP : yes
Test substance :

Source : Stickstoffwerke AG Lu. Wittenberg

Value : 213 - °C at
Decomposition : ambiguous
Method : other
Year : 1992
GLP : no data
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
Test substance : 100% H3PO4, see ref (2)

Value : = - 135 °C at
Decomposition :
Method : other
Year : 1998
GLP : no data
Test substance :

Source : See paragraph 1.04.
Leduc Chemie B.V. Amersfoort

2.3 DENSITY

Type : density
Value : = - 1.5788 g/cm? at 15 °C
Method : other
Year : 1998
GLP : no data
Test substance :

Source : See paragraph 1.04.
Leduc Chemie B.V. Amersfoort

Type : density
Value : = 1.57 - g/cm? at 20 °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphoräure 75 %ig

(9)

Type : density
Value : ca. 1.58 - 1.7 g/cm? at 20 °C
Method : other
Year :
GLP : yes
Test substance :

Source : Stickstoffwerke AG Lu. Wittenberg

Type : density
Value : = 1.63 - g/cm? at 20 °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphorsäure 80 %ig

(9)

Type : density
Value : = 1.69 - g/cm? at 20 °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
Test substance : Phosphorsäure rein 85 %
Die Angaben zur Reinheit beziehen sich auf die Handelsware und nicht auf produzierte H3PO4.

(9) (6)

Type : density
Value : = 1.69 - g/cm? at 20 °C

Source : Hoechst AG Frankfurt/Main
Test substance : Phosphorsaeure 85 %ig

(10) (7)

Type : density
Value : = 1.7 - g/cm? at 20 °C
Method : other
Year : 1994
GLP : no data
Test substance :

Source : Grande Paroisse SA Paris la Defense 5

(14)

Type : density
Value : = 1.7 - g/cm? at 20 °C

Source : BASF AG Ludwigshafen

(13)

Type : density
Value : ca. 1530 - 1570 kg/m3 at 20 °C
Method : other

Year	:	
GLP	:	no data
Test substance	:	
Source	:	Grande Paroisse SA Paris la Defense 5
Test substance	:	for aqueous solutions between 70 and 75% phosphoric acid as produced. Pure solutions at 25°C would have the following densities: 10% soln. 1052 kg/m3 50% soln. 1333 kg/m3 75% soln. 1574 kg/m3 80% soln. 1628 kg/m3 85% soln. 1685 kg/m3 100% soln.1874 kg/m3

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .038 - hPa at 20 °C
Decomposition	:	
Method	:	other (measured)
Year	:	
GLP	:	yes
Test substance	:	
Source	:	Stickstoffwerke AG Lu. Wittenberg
Value	:	ca. .95 - .75 hPa at 20 °C
Source	:	Grande Paroisse SA Paris la Defense 5
Test substance	:	for 70% and 75% aqueous solutions of phosphoric acid respectively
Value	:	= 2 - hPa at 20 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen
Test substance	:	Phosphorsäure rein 85 % Die Angaben zur Reinheit beziehen sich auf die Handelsware und nicht auf produzierte H3PO4.

(6)

Value	:	= 2 - hPa at 20 °C
Decomposition	:	
Method	:	other (measured)
Year	:	1944
GLP	:	no data
Test substance	:	
Source	:	Grande Paroisse SA Paris la Defense 5

(15)

Value	:	= 2 - hPa at 20 °C
Source	:	BASF AG Ludwigshafen (13)
Value	:	= 2 - hPa at 20 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main
Test substance	:	Phosphorsaeure 85 %ig (7)
Value	:	= 40 - hPa at 50 °C
Decomposition	:	
Method	:	other (measured)
Year	:	1944
GLP	:	no data
Test substance	:	
Source	:	Grande Paroisse SA Paris la Defense 5 (16)
Value	:	= 40 - hPa at 50 °C
Source	:	BASF AG Ludwigshafen (13)
Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

2.5 PARTITION COEFFICIENT

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	
Value	:	- at °C
pH value	:	= 1 -
concentration	:	1 g/l at 20 °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	miscible
Stable	:	
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen
Test substance	:	Phosphorsäure rein 85 % Die Angaben zur Reinheit beziehen sich auf die Handelsware und nicht auf produzierte H3PO4.

(9) (6)

Solubility in	:	
Value	:	- at °C
pH value	:	= - 1.4
concentration	:	1 vol% at 20 °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	of very high solubility
Stable	:	
Deg. product	:	
Method	:	other
Year	:	1998
GLP	:	no data
Test substance	:	
Remark	:	This product dissolves in water without limits.
Source	:	Leduc Chemie B.V. Amersfoort

Solubility in	:	
Value	:	- at °C
pH value	:	= 1.5 -
concentration	:	3.3 g/l at 25 °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Remark	:	Totally miscible with water
Source	:	Grande Paroisse SA Paris la Defense 5

Solubility in	:	
Value	:	- at °C
pH value	:	= 1 -
concentration	:	1 g/l at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	soluble (1000-10000 mg/L)
Stable	:	
Deg. product	:	
Method	:	other
Year	:	1994
GLP	:	no data
Test substance	:	
Source	:	Grande Paroisse SA Paris la Defense 5

(15)

Solubility in	:	
Value	:	- at °C
pH value	:	1 -
concentration	:	1 g/l at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	soluble (1000-10000 mg/L)
Stable	:	
Source	:	BASF AG Ludwigshafen

(13)

Solubility in	:	
Value	:	- at °C
pH value	:	= 1 -
concentration	:	1 g/l at 20 °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	miscible
Stable	:	
Source	:	Hoechst AG Frankfurt/Main
Test substance	:	Phosphorsaeure 85 %ig

(10) (7)

Solubility in	:	
Value	:	ca. 750 - 850 g/l at 20 °C
pH value	:	ca. 1.5 -
concentration	:	10 g/l at 20 °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	
Source	:	Stickstoffwerke AG Lu. Wittenberg

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	°C
Type	:	closed cup
Method	:	other: DIN 51584
Year	:	
GLP	:	
Test substance	:	
Remark	:	nicht brennbar
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(9)

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

Remark	:	not applicable ref BASF Sicherheitsblatt Phosphorsaeure 75% solution not flammable
Source	:	Grande Paroisse SA Paris la Defense 5

Remark : nicht anwendbar
Source : BASF AG Ludwigshafen

(13)

2.8 AUTO FLAMMABILITY

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

Remark : not applicable
ref BASF Sicherheitsblatt Phosphorsaeure 75% solution
not flammable
Source : Grande Paroisse SA Paris la Defense 5

Remark : nicht anwendbar
Source : BASF AG Ludwigshafen

(13)

2.9 FLAMMABILITY

Result : non flammable
Method : other
Year :
GLP : no data
Test substance :

Remark : Combustion by-products include oxides of phosphorus see fer (2)
not flammable;however flammable gas may form on contact withmetals
Source : Grande Paroisse SA Paris la Defense 5

Result : non flammable
Method : other: DIN 51584
Year :
GLP :
Test substance :

Source : Hoechst AG Frankfurt/Main
Test substance : Phosphorsaeure 85 %ig

(10)

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

2.10 EXPLOSIVE PROPERTIES

Result : not explosive
Method : other
Year : 1998
GLP : no data

Test substance :

Source : See paragraph 1.04.
Leduc Chemie B.V. Amersfoort

Result : not explosive
Method : other
Year :
GLP : no data
Test substance :

Remark : none; however flamable gas formation in contact with metals may give rise to explosive gas mixtures with air.
Source : Grande Paroisse SA Paris la Defense 5

2.11 OXIDIZING PROPERTIES

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

Remark : Kinematische Viskositaet bei 25 Grad C: 0.305 cm2/s
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(9)

Remark : Infolge starker intermolekularer Wasserstoffbrückenbildung können die physikalisch-chemischen Daten anderer Konzentrationen von den hier genannten Daten stark abweichen.
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(17)

Remark : Phosphoric acid is a clourless or lightly greenish liquid with a sharp characteristic odour.
Source : Leduc Chemie B.V. Amersfoort

Remark : All physical data were collected from general chemical litterature such as Ullmann or Kirk-Othmer encyclopedia, Condensed chemical dictionary (Hawley),The Merck Index, CRC hanbook of Chemistry and Physics, Dangerous properties of industrial chemicals (Sax) Handbook of reactive chemical hazards (Bretherick) etc
For regulatory limits on emissions and other information

theRTECS and HSDB files were used. Other information was also extracted from the Commission Criteria document for phosphoric acid
see references (1) (2) (3)

Source : Grande Paroisse SA Paris la Defense 5

(18)

Remark : Proton bridging changes due to dilution and variations in impurities contained in the product may strongly affect any physoco-chemical data given (4)

Source : Grande Paroisse SA Paris la Defense 5

(19)

Remark : Kinematische Viskositaet bei 25 Grad C: 0.305 cm2/s

Source : Hoechst AG Frankfurt/Main

(10)

Remark : Infolge starker intermolekularer Wasserstoffbrueckenbildung koennen die physikalisch-chemischen Daten anderer Konzentrationen von den hier genannten Daten stark abweichen.

Source : Hoechst AG Frankfurt/Main

(17)

Remark : Viskositaet bei 20 Grad C: 200 mPas (Methode: DIN 51562)

Source : Hoechst AG Frankfurt/Main

(20)

3.1.1 PHOTODEGRADATION

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

Remark : stable
Source : Grande Paroisse SA Paris la Defense 5

3.1.2 STABILITY IN WATER

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

Remark : undergoes ionic dissociation as any strong acid; may be reduced under anaerobic conditions by certain bacteria when suitably diluted
Source : Grande Paroisse SA Paris la Defense 5

3.1.3 STABILITY IN SOIL

Remark : Bildung von schwerlöslichen Phosphaten (z.B. CaHPO4); in dieser Form oder als lösliche Salze als Dünger pflanzenverfügbar.
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(21)

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

Remark : Phosphorus is a primary plant nutrient supplied to plants as PO4 ion component of Phosphoric acid
Phosphoric acid as such reacts chemically with soil components of alcaline type to form more or less soluble phosphate compounds depending on final pH.These compounds are mainly of the sparsely soluble calcium type which are used as fertilisers.
Under anaerobic conditions in presence of certain micro-organisms phosphate may undergo reduction to phosphine.
Source : Grande Paroisse SA Paris la Defense 5

Remark : Bildung von schwerloeslichen Phosphaten (z.B. CaHPO4); in dieser Form oder als loesliche Salze als Duenger pflanzenverfuegbar.
Source : Hoechst AG Frankfurt/Main

(21)

3.2.1 MONITORING DATA

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : other
Media : water - soil
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method :
Year :

Remark : under acidic soil conditions sparsely phosphates tend to solubilise and may migrate to water.
Source : Grande Paroisse SA Paris la Defense 5

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

3.3.2 DISTRIBUTION

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

3.4 MODE OF DEGRADATION IN ACTUAL USE

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

Remark : none
Source : Grande Paroisse SA Paris la Defense 5

3.5 BIODEGRADATION

Type : anaerobic
Inoculum : anaerobic microorganisms

Remark : under anaerobic conditions certain micro-organisms may degrade the product or related phosphates to phosphine.
Source : Grande Paroisse SA Paris la Defense 5

Type : anaerobic
Inoculum :

Remark : In anaeroben Systemen kann unter bestimmten Bedingungen H3PO4 zu P4 oder PH3 reduziert werden.
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(21)

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

3.6 BOD5, COD OR BOD5/COD RATIO

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

3.7 BIOACCUMULATION

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

Remark : Phosphates are normal body or skeleton components of practically all life forms.
Source : Grande Paroisse SA Paris la Defense 5

3.8 ADDITIONAL REMARKS

Remark : We have no additional remarks.
Source : Leduc Chemie B.V. Amersfoort

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96
Unit	:	
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	DL50 equivalent dose is reached between pH 3.0 and 3.5. Sublethal effects can be alreay noted at higher pH. The bluegill becomes hypoactive with respect to swimming behavior.
Source	:	Grande Paroisse SA Paris la Defense 5

(22)

Type	:	static
Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest an Fischen
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säure und im Vergleich verschiedener Säuren (H2SO4, HNO3, HCl, H3PO4) ermittelt werden. Die Anionen der getesteten Säuren spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH 3 - 3.5 (Phosphorsäure) Subletale Effekte schon bei höheren pH-Werten
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(23)

Type	:	static
Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest an Fischen
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeure und im Vergleich verschiedener Saeuren (H2SO4, HNO3, HCl, H3PO4) ermittelt werden. Die Anionen der getesteten Saeuren spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH 3 - 3.5 (Phosphorsaeure)

Subletale Effekte schon bei hoeheren pH-Werten
Source : Hoechst AG Frankfurt/Main

(23)

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

Type : other
Species : Gambusia affinis (Fish, fresh water)
Exposure period : 96 hour(s)
Unit :
LC50 : ca. 3 - 3.5
Limit test :
Analytical monitoring : no data
Method : other
Year :
GLP : no data
Test substance : other TS

Remark : The numbers are expressed as pH of the meduim whic does not directly give the concentration see ref (5)
Source : Grande Paroisse SA Paris la Defense 5

(24)

Type : other
Species :
Exposure period :
Unit :

Source : Stickstoffwerke AG Lu. Wittenberg

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 12 hour(s)
Unit :
EC50 : = 4.6 -
Analytical monitoring : yes
Method : other
Year : 1982
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : The survival rate depends on pH value generated by the acid:DL50 at pH 4.6
Source : Grande Paroisse SA Paris la Defense 5

(25)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark	:	Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säure ermittelt werden. Die Anionen der getesteten Säuren (z. B. Zitronensäure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH = 4.6 (Phorphorsäure)
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(26)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeure ermittelt werden. Die Anionen der getesteten Saeuren (z. B. Zitronensaeure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH = 4.6 (Phorphorsaeure)
Source	:	Hoechst AG Frankfurt/Main

(26)

Type	:	
Species	:	Daphnia pulex (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	the survival rate depends on the pH generated by the acid: DL50 at pH4.1 see ref (6)
Source	:	Grande Paroisse SA Paris la Defense 5

Type	:	
Species	:	Daphnia pulex (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säuren ermittelt werden. Die Anionen der getesteten Säuren (z. B. Zitronensäure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH = 4.1 (Phosphorsäure)
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(26)

Type	:	
Species	:	Daphnia pulex (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeuren ermittelt werden. Die Anionen der getesteten Saeuren (z. B. Zitronensaeure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH = 4.1 (Phosphorsaeure)
Source	:	Hoechst AG Frankfurt/Main

(26)

Type	:	
Species	:	Gammarus pulex (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
EC50	:	= 3.4 -
Analytical monitoring	:	yes
Method	:	other
Year	:	1982
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The survival rate depends on the pH value generated by the addition of acid to the media: DL50 at ph 3.4. The same applies to Gammarus fossarum. See ref (6)
Source	:	Grande Paroisse SA Paris la Defense 5

Type	:	
Species	:	Gammarus pulex (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säure ermittelt werden. Die Anionen der getesteten Säuren (z. B. Zitronensäure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalität bei pH 3.4 (Phosphorsäure)
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(26)

Type	:	
Species	:	Gammarus pulex (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse

Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeure ermittelt werden. Die Anionen der getesteten Saeuren (z. B. Zitronensaeure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH = 3.4 (Phosphorsaeure)
Source	:	Hoechst AG Frankfurt/Main

(26)

Type	:	
Species	:	other: Gammarus fossarum (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säure ermittelt werden. Die Anionen der getesteten Säuren (z. B. Zitronensäure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalität bei pH 3.4 (Phosphorsäure)
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(26)

Type	:	
Species	:	other: Gammarus fossarum (Crustacea)
Exposure period	:	12 hour(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeure ermittelt werden. Die Anionen der getesteten Saeuren (z. B. Zitronensaeure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH 3.4 (Phosphorsaeure)
Source	:	Hoechst AG Frankfurt/Main

(26)

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Remark	:	No information.

Source : Leduc Chemie B.V. Amersfoort

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic
Species : activated sludge
Exposure period :
Unit : mg/l
EC50 : = 270 -
Analytical monitoring : no
Method : other
Year :
GLP : no
Test substance :

Remark : The 270mg/l is equivalent to a pH of approximately 2.8 see ref (7). For other protozoa the level is 240 mg/l for DL50
Source : Grande Paroisse SA Paris la Defense 5

(27)

Type : aquatic
Species : activated sludge
Exposure period :
Unit : mg/l
EC50 : = 270 -
Analytical monitoring : no data
Method : other: Sauerstoffzehrungshemmtest
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Bericht in japanischer Sprache; Angaben aus Abstract, Tabellen- und Grafikbeschriftung in Englisch
270 mg/l ergeben einen pH-Wert von ca. 2.8
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(28) (29)

Type : aquatic
Species : other protozoa
Exposure period :
Unit : mg/l
LC50 : = 240 -
Analytical monitoring : no data
Method : other: Protozoa-Toxizitaetstest
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Bericht in japanischer Sprache; Angaben aus Abstract, Tabellen- und Grafikbeschriftung in Englisch
270 mg/l ergeben einen pH-Wert von ca. 2.8
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(28) (29)

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

4.5.1 CHRONIC TOXICITY TO FISH

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort
Species	:	other terrestrial plant
Endpoint	:	other
Exposure period	:	
Unit	:	
Method	:	other
Year	:	1992
GLP	:	no data
Test substance	:	other TS
Remark	:	The foliage of peas, beans, beets, rapeseed and weeds was destroyed when sprayed with 15-20% solution of phosphoric acid see ref (5)
Source	:	Grande Paroisse SA Paris la Defense 5

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

4.7 BIOLOGICAL EFFECTS MONITORING

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

4.8 BIOTRANSFORMATION AND KINETICS

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

4.9 ADDITIONAL REMARKS

Remark : Das ökotoxikologische Wirkungsprofil der Phosphorsäure wird geprägt durch:
1. Acidität (pH-Wert)
2. Phosphatbildung, mögliche Eutrophierung natürlicher Ökosysteme, z. B. "Algenblüte", mit toxischen Folgen für terrestrische und aquatische Organismen durch Sauerstoffzehrung absterbender Algen,

siehe auch Kapitel 1.1
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(11)

Result : Phosphoric acid acidifies ground and air and poisons plants and animals. These are the limits according to Polish regulations:
-Permissible pollution of surface inland waters:

	ph value	concentration of phosphate ion
1st class	6.5-8.0	0.2 mg/dm3
2nd class	6.5-9.0	0.5 mg/dm3
3rd class	6.0-9.0	1.0 mg/dm3

of purity
-Permissible contamination of waste entering internal and external sea waters:
content of phosphoric acid in sewages must be safe for human health and living sea organisms
-Permissible pollution of wastes taken off into sewage system:
ph value: 6.5-9.0.
Source : see paragraph 1.04.
Leduc Chemie B.V. Amersfoort

Remark : In the aquatic environment, the acid may affect the pH levelof the water body and the phosphate entity may persist indefinitely. The presence of phosphate in surface waters can produce a fertiliser action on algal growth and produce algal blooms which leads to aprocess called eutrophication. When phosphate acids or slats are spilled onto soil, they will infiltrate and migrate downward due to their high solubility. In the process they can dissolve some soil materials and be partially neutralised in the process. On reaching the ground table the acid will be dispersed and diluted. see ref (5).
Source : Grande Paroisse SA Paris la Defense 5

Remark : Das oekotoxikologische Wirkungsprofil der Phosphorsaeure

wird gepraegt durch:
1. Aciditaet (pH-Wert)
2. Phosphatbildung, moegliche Eutrophierung natuerlicher Oekosysteme, z. B. "Algenbluete", mit toxischen Folgen fuer terrestrische und aquatische Organismen durch Sauerstoffzehrung absterbender Algen,

siehe auch Kapitel 1.1

Source : Hoechst AG Frankfurt/Main

(11)

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1530 - mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other: keine Daten
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(30)

Type	:	LD50
Value	:	= - 1530 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1997
GLP	:	no data
Test substance	:	no data
Source	:	Bases on the specifications for UN-number 1805. Leduc Chemie B.V. Amersfoort

Type	:	LD50
Value	:	= 1530 - mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Grande Paroisse SA Paris la Defense 5

(31)

Type	:	LD50
Value	:	ca. 1530 - mg/kg bw
Species	:	rat
Strain	:	

Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Stickstoffwerke AG Lu. Wittenberg
Type	:	other
Value	:	-
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1992
GLP	:	no data
Test substance	:	no data
Remark	:	Although exposure to phosphoric acid may result in effects attribuable to the acid component, there is no evidence thatphohphorus poisoning can occur on exposure to phosphoric acid. see ref (5) FAO/WHO Expert Committee On Food Additives recommended levels for total dietary phosphorus level of less than 30mg/kg body wt is considered safe in any type of diet... Conditional acceptance level of30-70mg/kg is only aceptable when dietary calcium intake is high see ref (2)
Source	:	Grande Paroisse SA Paris la Defense 5
Type	:	other
Value	:	= 50 - 100 mg/kg bw
Species	:	sheep
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1973
GLP	:	no data
Test substance	:	no data
Remark	:	Doses of up to 50mg/kg bw/day administered in the drinking water produced no advers effects. Levels of 100mg/kg bw/day caused loss of weight and death see ref (3)
Source	:	Grande Paroisse SA Paris la Defense 5

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	= 1.689 - mg/l
Species	:	rabbit
Strain	:	
Sex	:	

Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	1 hour(s)
Method	:	other
Year	:	1981
GLP	:	no data
Test substance	:	no data
Remark	:	figure given is stated as being 1689 mg/m3 of P2O5 see ref (3) p55. Other data are given for rat:1217mg/m3;mouse 271mg/m3;guinea-pig 61mg/m3 allways as P2O5
Source	:	Grande Paroisse SA Paris la Defense 5

Type	:	LCLo
Value	:	= .1 - mg/l
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(32) (33)

Type	:	LCLo
Value	:	= .1 - mg/l
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	Grande Paroisse SA Paris la Defense 5

(34)

Type	:	other
Value	:	= 10 - mg/l
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other: Keine Angaben
Year	:	
GLP	:	no data
Test substance	:	no data

Remark	:	10 000 mg/m3 is considered immediately dangerous to life or health as classified by NIOSH Inhalation of mists of phosphoric acid can be irritating to the upper respiratory tract, however production of pulmonaryoedema is not likely
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(32)

Type	:	other
Value	:	= 10 - mg/l
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other
Year	:	1990
GLP	:	no data
Test substance	:	no data

Remark	:	10 000 mg/m3 is considered immediately dangerous to life or health as classified by NIOSH see ref (2) Inhalation of mists of phosphoric acid can be irritating to the upper respiratory tract, however production of pulmonaryoedema is not likely see ref (5)
Source	:	Grande Paroisse SA Paris la Defense 5

Type	:	other
Value	:	-
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Source	:	Stickstoffwerke AG Lu. Wittenberg

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	= 2740 - mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other: keine Daten
Year	:	
GLP	:	no data

Test substance	:	no data
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen

(30)

Type	:	LD50
Value	:	= - 2740 mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1997
GLP	:	no data
Test substance	:	no data
Source	:	Based on the specifications for UN-number 1805. Leduc Chemie B.V. Amersfoort
Type	:	LD50
Value	:	= 2740 - mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Grande Paroisse SA Paris la Defense 5

(31)

Type	:	LD50
Value	:	ca. 2730 - mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Stickstoffwerke AG Lu. Wittenberg
Type	:	LDLo
Value	:	= 2000 - 5010 mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other

Year	:	1976
GLP	:	no data
Test substance	:	other TS
Remark	:	The dermal ld50 for phosphoric acid 85%, 80, 75% were respectively >1260, >3160, >3160 and the LDLo were 2000, 5010, 5010. see ref (11) application was on albino rabbits, clipped skin, 24 hours
Source	:	Grande Paroisse SA Paris la Defense 5

(35)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LDLo
Value	:	= 220 - mg/kg bw
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Route of admin.	:	other
Exposure time	:	
Method	:	unreported
Year	:	
GLP	:	no data
Test substance	:	other TS
Source	:	Grande Paroisse SA Paris la Defense 5

(36)

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	not irritating
Classification	:	not irritating
Method	:	Draize Test
Year	:	1988
GLP	:	no data
Test substance	:	other TS
Remark	:	4 Stunden Expositionzeit Modified skin irritation test, White NZ rabbit, irritating assessment as non-irritating after Draize scoring 4.5-48 hours
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen
Test substance	:	Phosphoräure 75 %ig

(37)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	highly irritating
Classification	:	
Method	:	other: nach § 1500.41 in Federal Register 38, No. 187, p. 27029 vom 27.09.73
Year	:	1980
GLP	:	no
Test substance	:	other TS
Remark	:	6 Kaninchen (Weiße Wiener), Prüfung an intakter und skarifizierter Haut, Einwirkzeit 24 Stunden
Result	:	tiefgehende Nekrosen an der intakten Haut, primärer Reizwert= 6.6
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen
Test substance	:	ca. 80 %ige Phosphorsäure

(38)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	not irritating
Classification	:	
Method	:	other: keine Angaben
Year	:	1980
GLP	:	no
Test substance	:	other TS
Remark	:	2 Kaninchen (Weiße Wiener), Prüfung an der intakten Haut, Einwirkzeit 4 Stunden
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen
Test substance	:	19 %ige Phosphorsäure

(39)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	
Classification	:	
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1985
GLP	:	yes
Test substance	:	other TS
Result	:	2.5 %ige Phosphorsäure = nicht reizend

17.5 %ige Phosphorsäure = Nekrosen bei 1 von 3 Tieren
25 %ige Phosphorsäure = Nekrosen bei allen 3 Tieren
35 %ige Phosphorsäure = Nekrosen bei 1 von 3 Tieren

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

Test substance : siehe RS

(40)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result :
Classification :
Method :
Year :
GLP :
Test substance :

Remark : Dermal irritancy for different aqueous solutions was tested on rabbits including phosphoric acid. The irritation/corrosion was proportional to the concentration. see ref (9)

Source : Grande Paroisse SA Paris la Defense 5

(41)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : highly irritating
Classification : corrosive (causes burns)
Method : other
Year : 1977
GLP : no data
Test substance : other TS

Remark : BIOFAX Ind-Test Lab 17-4/70y terms as severe the effect observed on the skin of rabbit after treatment for 24h at 95mg of acid. No other data are given. see ref (1)

Source : Grande Paroisse SA Paris la Defense 5

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : corrosive
Classification : corrosive (causes burns)
Method : other
Year : 1977
GLP : no data
Test substance : other TS

Remark	:	Application of 0.5ml of commercial product to clipped skin of New Zealand albino rabbits under semi occlusive dressingsfor 24 hrs. Solutions from 75-85% phosphoric acid were corrosive to skin see ref (10)
Source	:	Grande Paroisse SA Paris la Defense 5

(42)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	irritating
Classification	:	irritating
Method	:	other
Year	:	1977
GLP	:	no data
Test substance	:	other TS

Remark	:	In the same test as in ref (10) on albino rabbits but only for 4 hours 75 and 80% phosphoric acid was considered as non-corrosive while 85% acid was corrosive. DOT skin corrosion classification.
Source	:	Grande Paroisse SA Paris la Defense 5

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	not irritating
Classification	:	not irritating
Method	:	Draize Test
Year	:	1988
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Remark	:	Modified skin irritation test, White NZ rabbit, 75% phosphoric acid, 4hours contact, irritation assessment non-irritating after Draize scoring 4.5-48 hours. see ref (11)
Source	:	Grande Paroisse SA Paris la Defense 5

(43)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	highly irritating
Classification	:	
Method	:	other: Federal Register 38,n°187 & 1500.41. p.27029 (27.09.73)
Year	:	1980
GLP	:	no
Test substance	:	other TS

Remark : Test substance 80% solution
Source : Grande Paroisse SA Paris la Defense 5

(44)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : not irritating
Classification :
Method : other
Year : 1980
GLP : no
Test substance : other TS

Remark : Test substance other: 19% solution
Source : Grande Paroisse SA Paris la Defense 5

(45)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : highly irritating
Classification :
Method : other: nach Federal Register 38, No.187, Para. 1500.41, S. 27029, vom 27.09.1973
Year :
GLP : no
Test substance : other TS

Source : BASF AG Ludwigshafen
Test substance : Phosphorsaeure, ca. 80 %ig

(46)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : not irritating
Classification :
Method : other: BASF-Test
Year :
GLP : no
Test substance : other TS

Source : BASF AG Ludwigshafen
Test substance : Phosphorsaeure, 19 %ig

(47)

Species : rabbit
Concentration :
Exposure :

Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	not irritating
Classification	:	not irritating
Method	:	Draize Test
Year	:	1988
GLP	:	no data
Test substance	:	other TS
Remark	:	4 Stunden Expositionzeit Modified skin irritation test, White NZ rabbit, irritatiing assessment non-irritating after Draize scring 4.5-48 hours
Source	:	Hoechst AG Frankfurt/Main
Test substance	:	Phosphoraeure 75%ig

(37)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	highly irritating
Classification	:	
Method	:	other: federal Register 38.n 187 & 1500.41.p.27029 (27.09.73)
Year	:	
GLP	:	no
Test substance	:	other TS
Source	:	Hoechst AG Frankfurt/Main
Test substance	:	80 %ige Loesung

(48)

Species	:	other
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	highly irritating
Classification	:	
Method	:	Estimation
Year	:	
GLP	:	
Test substance	:	other TS
Remark	:	The method used is the predictive Buchner (1979) method forjudging irritative potentials of chemicals.Test substance was 30% H3PO4. In a parallel estimate 5% H3PO4 was considered to be moderately irritating.
Source	:	Grande Paroisse SA Paris la Defense 5

(49)

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	
Vehicle	:	
Result	:	not irritating
Classification	:	not irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1988
GLP	:	yes
Test substance	:	other TS
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen
Test substance	:	10 und 17%ige Phosphorsäure

(50)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	
Vehicle	:	
Result	:	irritating
Classification	:	risk of serious damage to eyes
Method	:	other
Year	:	1970
GLP	:	no data
Test substance	:	no data
Remark	:	BIOFAX Ind Bio-Test Lab 17-4/70 states as severe the effectsobserved on rabbit's eyes with a dose of 119mg. No other data are given. see ref (1) and (3)
Source	:	Grande Paroisse SA Paris la Defense 5

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	
Vehicle	:	
Result	:	not irritating
Classification	:	not irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1988
GLP	:	yes
Test substance	:	other TS
Remark	:	Two dilutions of phosphoric acid have been tested on N.Z white albino rabbits: 10 and 17% and scored following Draizescoring criteria and finally classified by EC criteria as "not irritating to eyes". see ref (12)
Source	:	Grande Paroisse SA Paris la Defense 5

(51)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	
Vehicle	:	
Result	:	not irritating
Classification	:	not irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1988
GLP	:	yes
Test substance	:	other TS
Source	:	Hoechst AG Frankfurt/Main
Test substance	:	10 und 17%ige Phosphorsaeure

(50)

Species	:	human
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	
Vehicle	:	
Result	:	irritating
Classification	:	irritating
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	other TS
Remark	:	Contact with eyes may cause irritation and burns. it has been classified as irritant by EC directive see ref (3)This is in FORMAL contradiction with ref (12)! which see Phosphoric acid has low vapour pressure at room temperature;does not produce eye irritetion unless it is present as spray or mist. Dilute solutions buffered to pH 2.5 only caused a transient stinging sensation when placed directly into the eye; acclimated workers can easily tolerate permissible exposure limits. see ref (5)
Source	:	Grande Paroisse SA Paris la Defense 5
Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

5.3 SENSITIZATION

Type	:	no data
Species	:	human
Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Remark	:	no sensitization potential of phosphates or phosphoric acid was found. See ref (5)
Source	:	Grande Paroisse SA Paris la Defense 5

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

5.4 REPEATED DOSE TOXICITY

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

5.5 GENETIC TOXICITY 'IN VITRO'

Remark	:	No information.
Source	:	Leduc Chemie B.V. Amersfoort

Type	:	Salmonella typhimurium reverse mutation assay
System of testing	:	
Test concentration	:	various concentrations for food
Cycotoxic concentr.	:	
Metabolic activation	:	no data
Result	:	negative
Method	:	other
Year	:	
GLP	:	
Test substance	:	

Remark	:	4 acidity regulators including phosphoric acid have been tested. None of the samples tested was mutagenic. see ref (13)
Source	:	Grande Paroisse SA Paris la Defense 5

(52)

Type	:	Salmonella typhimurium reverse mutation assay
System of testing	:	
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	negative
Method	:	other
Year	:	1986
GLP	:	no data
Test substance	:	other TS

Remark	:	No effects were detectable in S.typhimurium tester strains following sublethal pH decrease. (see ref 13 and 3)
Source	:	Grande Paroisse SA Paris la Defense 5

(53)

5.6 GENETIC TOXICITY 'IN VIVO'

Remark	:	No information.

Source : Leduc Chemie B.V. Amersfoort

5.7 CARCINOGENICITY

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

5.8.1 TOXICITY TO FERTILITY

Type : One generation study
Species : rat
Sex : no data
Strain : no data
Route of admin. : oral feed
Exposure period :
Frequency of treatm. : diets containing 0.75%(375mg/kgbw/d) no harmful effect
Premating exposure period
Male :
Female :
Duration of test : 29 wk
No. of generation studies :
Doses : 180-375mg/kgbw/d
Control group :

Remark : see ref (5)The higher dietary level of 0.75%PA (375mg/kgbw/d) apparently had no harmful effect on growth ofoffspring
Source : Grande Paroisse SA Paris la Defense 5

Type : other
Species : Chinese hamster
Sex : no data
Strain : other
Route of admin. :
Exposure period :
Frequency of treatm. :
Premating exposure period
Male :
Female :
Duration of test :
No. of generation studies :
Doses :
Control group :

Remark : Effects of phosphoric acid on the growth, survival rate and macromolecular synthesis of mammalian cells of the Chinese hamster V79 lung cells that has been examined as themeasure of the product cytotoxicity. All effect appeared suddenly at or above 30mM in a short time.see ref (14)
Source : Grande Paroisse SA Paris la Defense 5

(54)

Type : other
Species : human
Sex : no data

Strain	:	
Route of admin.	:	
Exposure period	:	
Frequency of treatm.	:	
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	
No. of generation studies	:	
Doses	:	
Control group	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	no data

Remark : No information was located on the reproductive toxic potential of phosphoric acid or phosphatess. see ref (5)
Source : Grande Paroisse SA Paris la Defense 5

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

Remark : Proband, 5 ml einer 1.0 %igen Phosphorsäurelösung, p.o., Expositionsdauer 5 s
Wirkung:
Keine Ösophagusverätzung
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen

(55)

Result : This product is strongly caustic and irritates eyes, muscousmembranes, tissues and skin. Intoxication by acid may cause local and overall injuries. Basic result of poisining is damage of tissues. In case of eye contact: conjunctivis and keratitis; pain, tears and photophobia. In case of ingestion: strong and acute pain of oral cavity, throat, esophagus, stomach and abdominal cavity; coughing and vomiting, often with blood and brown content; perforation

ofesophagus, stomach and sometimes intestines may occur.

Source : Leduc Chemie B.V. Amersfoort

Remark : Recommended threshold limit is based by analogy from comparable experience and data for sulfuric acid. Fumes ofphosphorus pentoxide at concentrations from 0.8 to 5.4 mg/m3 are noticeable but not uncomfortable and concentrations between 3.6 and 11.3 mg/m3 caused coughing among inexperienced but could be tolerated. Concentrations of 100mg/m3 were unendurable except for hardened workers. TLV of 1mg/m3 is accordingly below the concentration that causes throat irritation among unacclimated workers and wellbelow that which is well tolerated by acclimated workers. See ref (2)
There is no evidence that chronic phosphorus poisoning results from contact with phosphoric acid. Phosphoric acid is considerably less harmful than sulphuric, hydrochloric ornitric acids. See ref (5)

Source : Grande Paroisse SA Paris la Defense 5

Remark : Es liegen keine Untersuchungsberichte der BASF vor.

Source : BASF AG Ludwigshafen

Remark : Proband, 5 ml einer 1.0 %igen Phosphorsaeureloesung, p.o., Expositionsdauer 5 s
Wirkung:
Keine Oesophagusveraetzung

Source : Hoechst AG Frankfurt/Main

(55)

5.11 ADDITIONAL REMARKS

Type : Neurotoxicity

Remark : It seems that very high doses lead to physiological disturbances translated as phosphate toxicity which can produce central nervous system involvement which is manifested by convulsions , delirium and coma. See ref (5) and (3)

Source : Grande Paroisse SA Paris la Defense 5

Remark : We have no other relevant information.

Source : Leduc Chemie B.V. Amersfoort

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) TRGS 900 (1993)

(2) ACGIH (1991-1992)

(3) (1)

(4) Ministerium SZW (1996): Die Nationale MAC-Liste (11ed. 1996)

(5) Bundesminister des Innern (1990): Gemeinsames Ministerialblatt Nr. 124, Kenn-Nr. 392 (23.03.1990)

(6) ThermPhos International (1997): Sicherheitsdatenblatt Phosphorsäure rein 85 %

(7) Hoechst AG (1994): Sicherheitsdatenblatt Phosphorsaeure rein 85 prozentig (27.04.1994)

(8) Stoerfall-Verordnung vom 20.09.1991

(9) ThermPhos International (1997): Produktinformation Phosphorsäure

(10) Hoechst AG (1991): Produktinformation Phosphorsaeure der Abt. Marketing Chemikalien (Februar 1991)

(11) US-EPA (1990): Fed. Regist. 55(122), 25876-25878 (25.06.1990)

(12) boiling point > 135°C at atmospheric pressure for a 75% solution as given by BASF Sicherheitsdatenblatt Phosphorsaeure.

(13) BASF AG, Sicherheitsdatenblatt Phosphorsaeure (12/90). Bezieht sich auf 75 %ige H3PO4.

(14) BASF Sicherheitsblatt Phosphorsaeure 75% aqueous solution

(15) BASF Sicherheitsblatt Phosphorsaeure 75% solution

(16) BASF sicherheitsblatt Phosphorsaeure 75% solution

(17) Hollemann-Wiberg (1976): Lehrbuch der anorganischen Chemie, Berlin, New York, 449

(18) (1) RTECS AN NIOSH TB 6300000 RN 7664-38-2
(2) HSDB AN 001187 (Hazardous Substance Data Bank)
(3) Occupational Exposure Limits, Criteria document for Phosphoric acid, Report EUR 14178 EN, 1992

(19) (4) Hollerman-Viberg, 1976: Lehrbuch der anorganischen Chemie, p.449

(20) Hoechst AG (1993): Produktinformation Knapsack-Reinigerkomponente MS der Abt. Marketing Chemikalien (19.10.1993)

(21) Hoechst AG (1992): Interne Mitteilung der Abt. F+E Chemikalien (09.09.1992)

(22) (4) Ellgaard,E.G. Gilmore,J.Y.Jr. 1984, J. Fish Biol. 25 (2)133-7, see also ref (2)

(23) Ellgaard, Gilmore (1984): J. Fish Biol. 25(2), 133-137

(24) (5) Phosphoric acid/phosphates a Review, Von Burg, R.,J. Appl. Tox. 12, (4), 301-3, 1992.

(25) (6) Brehm, Meijerling, Arch Hydrobiol 95, (1-4) 17-27, 1982

(26) Brehm, Meijering (1982): Arch. Hydrobiol. 95(1-4), 17-27

(27) (7)Iishi,Kaji, Noguchi, 1981, Suishitsu Odaku Kengyu 4 (4) 197-203 abstract and figures only

(28) Hoechst AG (1992): Information der Abt. Analytisches Laboratorium (11.08.1992)

(29) Ishi, Kaji, Noguchi (1981): Suishitsu Odaku Kenkyu 4(4), 197-203

(30) BIOFAX Ind. (1970): Bio-Test Lab. 17-4/70; zitiert in: RTECS (1991)

(31) see ref (1)

(32) HSDB AN 001187 (Hazardous Substance Data Bank)

(33) SAX: Dangerous properties of industrial Material

(34) see ref (2) and also Dangerous properties of industrial Materials, Sax.

(35) (11) Acute toxic evaluation of various concentrations of phosphoric acid, Randall,D.J., Robinson, E.C., Acute toxic. data, 1 (1), 69-70, 1990

(36) see ref (1) and ref (3)p.55

(37) Weiner et al (1990): Acute Toxic. data 1 (2), 98-9

(38) BASF AG (1980): Unveröffentl. Unters. Ber. 79/322

(39) BASF AG (1980): Unveröffentl. Unters. Ber. 79/412

(40) Loden et al. (1985): FOA-Bericht, E40023 (Forschungsanstalt der Landesverteidigung) Umea, Schweden.

(41) (9) Dermal irritancy/corrosion of 20 compounds in aqueous solutions Report FOA-E-40023 Avail NTIS Gov. Rep. Index (US)1986, 86 (7), Abstr. n° 613 483, 1985

(42) (10) Skin irritation tests on various concentrations of phosphoric acid, Randall, D.J., Robinson, E.C., Acute Tox. Data 1 (1), 68-9, 1990

(43) (11) Modified skin irritation study on 75% phosphoric acid in a single rabbit, Weiner, M., Freeman, C., et al, Acute Toxic. data, 1 (2), 98-9, 1990

(44) BASF AG Abt Toxicologie, unveroffentlichte Untesuchung (79/322) 06.05.1980

(45) BASF AG Abt. Toxicologie, unveroffentlichte Untersuchung, (79/412) 06.05.1980

(46) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, (79/322), 06.05.1980

(47) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, (79/412), 06.05.1980

(48) BASF AG (1980): Unveroeffentlichte Untersuchung (79/322)

(49) (8) The topically irritant substance:essentials- bio-tests -predictions, Buchner, K., Bucher, K.E., Walz, D., Agents Actions, 11 (5), 515-9, 1981

(50) Jacobs (1992): J. Am. Coll. Toxicol. 11, (6), 724

(51) (12) Two dilutions of phosphoric acid tested on the eye, Jacobs, G. A., J. Am. Coll Toxicol. 11, (6), 724, 1992

(52) (13) Al Ani,F.Y., Al Lami, S.K., Absence of mutagenic activity of acidity regulators in the Ames/samonella test, Mutat. Res., 206, (4), 467-70, 1988.

(53) (13) Sublethal pH decrease may cause genetic damage to eucaryotic cell: a study on sea urchins and S. typhimurium, Cipollaro, M. Corsale, G. et al, Terato, carcio, mutagenesis6, 275-87, 1986

(54) (14) Cytotoxicity of phosphoric acid on cultured mammalian cells, Iijima, Horii, Kanemaki et al, Shigaku, 80, (5) 1159-65, 1993

(55) von Muehlendahl et al. (1978): Arch. Toxicol. 39, 299-314

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-16174B

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IUCLID

Data Set

Existing Chemical	:	ID: 7664-38-2
CAS No.	:	7664-38-2
EINECS Name	:	orthophosphoric acid
EC No.	:	231-633-2
TSCA Name	:	Phosphoric acid
Molecular Formula	:	H3O4P

Producer related part

Company	:	Rhodia UK limited
Creation date	:	04.07.2005

Substance related part

Company	:	Rhodia UK limited
Creation date	:	04.07.2005
Status	:	
Memo	:	Rhodia new repro
Printing date	:	04.07.2005
Revision date	:	
Date of last update	:	04.07.2005
Number of pages	:	35
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value : ca. -20 - 0 °C
Decomposition : no, at - °C
Sublimation : no
Method : other
Year :
GLP :
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : melting point for aqueous solutions between 75 and 80% phosphoric acid as produced. Pure phosphoric acid solutions may differ due to absence of impurities ie.:
75% soln. - 17.5°C
80% soln. + 4.6°C
85% soln. + 21°C
18.02.1994

Value : = -20 - °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphoräure 75 %ig
09.10.1997 (1)

Value : = 3 - °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsäure 80 %ig
09.10.1997 (1)

Value : = 21 - °C

Remark : Erstarrungspunkt
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsäure rein 85 %
Die Angaben zur Reinheit beziehen sich auf die Handelsware und nicht auf produzierte H3PO4.
09.10.1997 (1) (2)

Value : = 21 - °C

Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsaeure 85 %ig
31.05.1994 (3) (4)

Value : = 42.4 - °C

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : Phosphorsäure kristallin
09.10.1997 (5)

Value : 42.4 - °C
Sublimation :
Method : other
Year : 1989
GLP : no
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : 100% H3PO4, see ref (2)
18.02.1994

Value : = 42.4 - °C

Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsaeure kristallin
11.08.1992 (5)

Value : = - -17.5 °C
Decomposition : no, at - °C
Sublimation : no
Method : other
Year : 1998
GLP : no data
Test substance :

Source : Based on a rapport from our Polish supplier (see paragraph 1.04).
Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.12.1998

2.2 BOILING POINT

Value : ca. 133 - °C at 1013 hPa
Decomposition : ambiguous
Method :
Year :
GLP :
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : 75% aqueous solution of phosphoric acid
29.04.1994

Value : = 135 - °C at 1013 hPa

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphoräure 75 %ig
09.10.1997 (1)

Value : > 135 - °C at 1013 hPa
Decomposition :

Method : other
Year : 1994
GLP : no data
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
29.04.1994 (6)

Value : > 135 - °C at

Source : BASF AG Ludwigshafen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
12.01.1994 (7)

Value : = 145 - °C at 1013 hPa

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsäure 80 %ig
09.10.1997 (1)

Value : = 158 - °C at 1013 hPa

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsäure rein 85 %
Die Angaben zur Reinheit beziehen sich auf die Handelsware
und nicht auf produzierte H3PO4.
09.10.1997 (1) (2)

Value : = 158 - °C at 1013 hPa

Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsaeure 85 %ig
31.05.1994 (3) (4)

Value : ca. 158 - °C at
Decomposition :
Method : other
Year :
GLP : yes
Test substance :

Source : Stickstoffwerke AG Lu. Wittenberg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.05.1994

Value : 213 - °C at
Decomposition : ambiguous
Method : other
Year : 1992
GLP : no data
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : 100% H3PO4, see ref (2)
18.02.1994

Value : = - 135 °C at
Decomposition :
Method : other
Year : 1998
GLP : no data
Test substance :

Source : See paragraph 1.04.
Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

2.4 VAPOUR PRESSURE

Value : = .038 - hPa at 20 °C
Decomposition :
Method : other (measured)
Year :
GLP : yes
Test substance :

Source : Stickstoffwerke AG Lu. Wittenberg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

11.05.1994

Value : ca. .95 - .75 hPa at 20 °C

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : for 70% and 75% aqueous solutions of phosphoric acid respectively

17.08.1993

Value : = 2 - hPa at 20 °C
Decomposition :
Method :
Year :
GLP : no data
Test substance :

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsäure rein 85 %
Die Angaben zur Reinheit beziehen sich auf die Handelsware und nicht auf produzierte H3PO4.

09.10.1997 (2)

Value : = 2 - hPa at 20 °C
Decomposition :
Method : other (measured)
Year : 1944
GLP : no data
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

29.04.1994 (8)

Value : = 2 - hPa at 20 °C

Source : BASF AG Ludwigshafen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
12.01.1994 (7)

Value : = 2 - hPa at 20 °C
Decomposition :
Method :
Year :
GLP : no data
Test substance :

Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsaeure 85 %ig
31.05.1994 (4)

Value : = 40 - hPa at 50 °C
Decomposition :
Method : other (measured)
Year : 1944
GLP : no data
Test substance :

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
29.04.1994 (9)

Value : = 40 - hPa at 50 °C

Source : BASF AG Ludwigshafen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
12.01.1994 (7)

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.12.1998

2.5 PARTITION COEFFICIENT

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.12.1998

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in :
Value : - at °C
pH value : = 1 -
concentration : 1 g/l at 20 °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C

Description : miscible
Stable :

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsäure rein 85 %
Die Angaben zur Reinheit beziehen sich auf die Handelsware
und nicht auf produzierte H3PO4.

09.10.1997 (1) (2)

Solubility in :
Value : - at °C
pH value : = - 1.4
concentration : 1 vol% at 20 °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : of very high solubility
Stable :
Deg. product :
Method : other
Year : 1998
GLP : no data
Test substance :

Remark : This product dissolves in water without limits.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

Solubility in :
Value : - at °C
pH value : = 1.5 -
concentration : 3.3 g/l at 25 °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Remark : Totally miscible with water
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

12.10.1993

Solubility in :
Value : - at °C
pH value : = 1 -
concentration : 1 g/l at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : soluble (1000-10000 mg/L)
Stable :
Deg. product :
Method : other
Year : 1994
GLP : no data
Test substance :

Source : Grande Paroisse SA Paris la Defense 5

EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
29.04.1994 (8)

Solubility in :
Value : - at °C
pH value : 1 -
concentration : 1 g/l at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : soluble (1000-10000 mg/L)
Stable :

Source : BASF AG Ludwigshafen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
12.01.1994 (7)

Solubility in :
Value : - at °C
pH value : = 1 -
concentration : 1 g/l at 20 °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : miscible
Stable :

Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Phosphorsaeure 85 %ig
31.05.1994 (3) (4)

Solubility in :
Value : ca. 750 - 850 g/l at 20 °C
pH value : ca. 1.5 -
concentration : 10 g/l at 20 °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other
Year :
GLP : yes
Test substance :

Source : Stickstoffwerke AG Lu. Wittenberg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.05.1994

3.1.1 PHOTODEGRADATION

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

Remark : stable
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

14.10.1993

3.1.2 STABILITY IN WATER

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

Remark : undergoes ionic dissociation as any strong acid; may be reduced under anaerobic conditions by certain bacteria when suitably diluted
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

14.10.1993

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : other
Media : water - soil
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method :
Year :

Remark : under acidic soil conditions sparsely phosphates tend to solubilise and may migrate to water.
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

3.5 BIODEGRADATION

Type : anaerobic
Inoculum : anaerobic microorganisms

Remark : under anaerobic conditions certain micro-organisms may degrade the product or related phosphates to phosphine.
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994

Type : anaerobic
Inoculum :

Remark : In anaeroben Systemen kann unter bestimmten Bedingungen H_3PO_4 zu P_4 oder PH_3 reduziert werden.
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

11.09.1992 (10)

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Lepomis macrochirus (Fish, fresh water)
Exposure period : 96
Unit :
Limit test :
Analytical monitoring : yes
Method : other
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : DL50 equivalent dose is reached between pH 3.0 and 3.5. Sublethal effects can be alreay noted at higher pH. The bluegill becomes hypoactive with respect to swimming behavior.
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
18.02.1994 (11)

Type : static
Species : Lepomis macrochirus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit :
Limit test :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest an Fischen
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säure und im Vergleich verschiedener Säuren (H2SO4, HNO3, HCl, H3PO4) ermittelt werden. Die Anionen der getesteten Säuren spielten bei den getesteten Konzentrationen eine untergeordnete Rolle.
50 % Mortalitaet bei pH 3 - 3.5 (Phosphorsäure)
Subletale Effekte schon bei höheren pH-Werten
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
09.10.1997 (12)

Type : static
Species : Lepomis macrochirus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit :
Limit test :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest an Fischen
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeure und im Vergleich verschiedener Saeuren (H2SO4, HNO3, HCl, H3PO4) ermittelt werden. Die Anionen der getesteten Saeuren spielten bei den

getesteten Konzentrationen eine untergeordnete Rolle.
50 % Mortalitaet bei pH 3 - 3.5 (Phosphorsaeure)
Subletale Effekte schon bei hoeheren pH-Werten

Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

19.08.1992 (12)

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

Type : other
Species : Gambusia affinis (Fish, fresh water)
Exposure period : 96 hour(s)
Unit :
LC50 : ca. 3 - 3.5
Limit test :
Analytical monitoring : no data
Method : other
Year :
GLP : no data
Test substance : other TS

Remark : The numbers are expressed as pH of the meduim whic does not directly give the concentration see ref (5)
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (13)

Type : other
Species :
Exposure period :
Unit :

Source : Stickstoffwerke AG Lu. Wittenberg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

11.05.1994

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 12 hour(s)
Unit :
EC50 : = 4.6 -
Analytical monitoring : yes
Method : other
Year : 1982
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : The survival rate depends on pH value generated by the acid:DL50 at pH 4.6
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (14)

Type :

Species : Daphnia magna (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säure ermittelt werden. Die Anionen der getesteten Säuren (z. B. Zitronensäure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH = 4.6 (Phorphorsäure)
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

09.10.1997 (15)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeure ermittelt werden. Die Anionen der getesteten Saeuren (z. B. Zitronensaeure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH = 4.6 (Phorphorsaeure)
Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

13.08.1992 (15)

Type :
Species : Daphnia pulex (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : the survival rate depends on the pH generated by the acid: DL50 at pH4.1 see ref (6)
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994

Type :
Species : Daphnia pulex (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse

Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säuren ermittelt werden. Die Anionen der getesteten Säuren (z. B. Zitronensäure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle.
50 % Mortalitaet bei pH = 4.1 (Phosphorsäure)
Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
09.10.1997 (15)

Type :
Species : Daphnia pulex (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeuren ermittelt werden. Die Anionen der getesteten Saeuren (z. B. Zitronensaeure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle.
50 % Mortalitaet bei pH = 4.1 (Phosphorsaeure)
Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
13.08.1992 (15)

Type :
Species : Gammarus pulex (Crustacea)
Exposure period : 12 hour(s)
Unit :
EC50 : = 3.4 -
Analytical monitoring : yes
Method : other
Year : 1982
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : The survival rate depends on the pH value generated by the addition of acid to the media: DL50 at ph 3.4. The same applies to Gammarus fossarum. See ref (6)
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
18.02.1994

Type :
Species : Gammarus pulex (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säure ermittelt werden. Die Anionen der getesteten Säuren (z. B. Zitronensäure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalität bei pH 3.4 (Phosphorsäure)

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

09.10.1997 (15)

Type :
Species : Gammarus pulex (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeure ermittelt werden. Die Anionen der getesteten Saeuren (z. B. Zitronensaeure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalitaet bei pH = 3.4 (Phosphorsaeure)

Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

13.08.1992 (15)

Type :
Species : other: Gammarus fossarum (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Überlebensrate in Abhängigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Säure ermittelt werden. Die Anionen der getesteten Säuren (z. B. Zitronensäure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle. 50 % Mortalität bei pH 3.4 (Phosphorsäure)

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

09.10.1997 (15)

Type :
Species : other: Gammarus fossarum (Crustacea)
Exposure period : 12 hour(s)
Unit :
Analytical monitoring : yes
Method : other: Saeureempfindlichkeitstest auf ausgewaehlte Suesswasserkrebse
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Es sollte die Ueberlebensrate in Abhaengigkeit vom pH-Wert durch dem Versuchsmedium zugesetzte Saeure ermittelt werden. Die Anionen der getesteten Saeuren (z. B. Zitronensaeure) spielten bei den getesteten Konzentrationen eine untergeordnete Rolle.
50 % Mortalitaet bei pH 3.4 (Phosphorsaeure)

Source : Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

13.08.1992 (15)

Remark : No information.

Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Remark : No information.

Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1530 - mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other: keine Daten
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

13.08.1992 (16)

Type	:	LD50
Value	:	= - 1530 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1997
GLP	:	no data
Test substance	:	no data
Source	:	Bases on the specifications for UN-number 1805. Leduc Chemie B.V. Amersfoort EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

Type	:	LD50
Value	:	= 1530 - mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (17)

Type	:	LD50
Value	:	ca. 1530 - mg/kg bw
Species	:	rat
Strain	:	

Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Stickstoffwerke AG Lu. Wittenberg EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

11.05.1994

Type	:	other
Value	:	-
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1992
GLP	:	no data
Test substance	:	no data
Remark	:	Although exposure to phosphoric acid may result in effects attribuable to the acid component, there is no evidence thatphohphorus poisoning can occur on exposure to phosphoric acid. see ref (5) FAO/WHO Expert Committee On Food Additives recommended levels for total dietary phosphorus level of less than 30mg/kg body wt is considered safe in any type of diet... Conditional acceptance level of30-70mg/kg is only aceptable when dietary calcium intake is high see ref (2)
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994

Type	:	other
Value	:	= 50 - 100 mg/kg bw
Species	:	sheep
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1973
GLP	:	no data
Test substance	:	no data
Remark	:	Doses of up to 50mg/kg bw/day administered in the drinking water produced no advers effects. Levels of 100mg/kg bw/day caused loss of weight and death see ref (3)
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	= 1.689 - mg/l
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	1 hour(s)
Method	:	other
Year	:	1981
GLP	:	no data
Test substance	:	no data
Remark	:	figure given is stated as being 1689 mg/m3 of P2O5 see ref (3) p55. Other data are given for rat:1217mg/m3;mouse 271mg/m3;guinea-pig 61mg/m3 allways as P2O5
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994

Type	:	LCLo
Value	:	= .1 - mg/l
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

06.06.1994 (18) (19)

Type	:	LCLo
Value	:	= .1 - mg/l
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (20)

Type	:	other

Value	:	= 10 - mg/l
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other: Keine Angaben
Year	:	
GLP	:	no data
Test substance	:	no data
Remark	:	10 000 mg/m3 is considered immediately dangerous to life or health as classified by NIOSH Inhalation of mists of phosphoric acid can be irritating to the upper respiratory tract, however production of pulmonaryoedema is not likely
Source	:	Hoechst AG Frankfurt/Main ThermPhos International B.V. AK Vlissingen EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

06.06.1994 (18)

Type	:	other
Value	:	= 10 - mg/l
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other
Year	:	1990
GLP	:	no data
Test substance	:	no data
Remark	:	10 000 mg/m3 is considered immediately dangerous to life or health as classified by NIOSH see ref (2) Inhalation of mists of phosphoric acid can be irritating to the upper respiratory tract, however production of pulmonaryoedema is not likely see ref (5)
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994

Type	:	other
Value	:	-
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Source	:	Stickstoffwerke AG Lu. Wittenberg EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

11.05.1994

Remark : No information.

Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : = 2740 - mg/kg bw
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data

Source : Hoechst AG Frankfurt/Main
ThermPhos International B.V. AK Vlissingen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

13.08.1992 (16)

Type : LD50
Value : = - 2740 mg/kg bw
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other
Year : 1997
GLP : no data
Test substance : no data

Source : Based on the specifications for UN-number 1805.
Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

Type : LD50
Value : = 2740 - mg/kg bw
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (17)

Type : LD50

Value	:	ca. 2730 - mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Stickstoffwerke AG Lu. Wittenberg EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

11.05.1994

Type	:	LDLo
Value	:	= 2000 - 5010 mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1976
GLP	:	no data
Test substance	:	other TS
Remark	:	The dermal ld50 for phosphoric acid 85%, 80, 75% were respectively >1260, >3160, >3160 and the LDLo were 2000, 5010, 5010. see ref (11) application was on albino rabbits, clipped skin, 24 hours
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (21)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LDLo
Value	:	= 220 - mg/kg bw
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Route of admin.	:	other
Exposure time	:	
Method	:	unreported
Year	:	
GLP	:	no data
Test substance	:	other TS
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (22)

Remark	:	No information.

Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

5.4 REPEATED DOSE TOXICITY

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

5.5 GENETIC TOXICITY 'IN VITRO'

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

Type : Salmonella typhimurium reverse mutation assay
System of testing :
Test concentration : various concentrations for food
Cycotoxic concentr. :
Metabolic activation : no data
Result : negative
Method : other
Year :
GLP :
Test substance :

Remark : 4 acidity regulators including phosphoric acid have been tested. None of the samples tested was mutagenic. see ref (13)
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (23)

Type : Salmonella typhimurium reverse mutation assay
System of testing :
Test concentration :
Cycotoxic concentr. :
Metabolic activation :
Result : negative
Method : other
Year : 1986
GLP : no data
Test substance : other TS

Remark : No effects were detectable in S.typhimurium tester strains following sublethal pH decrease. (see ref 13 and 3)
Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (24)

5.6 GENETIC TOXICITY 'IN VIVO'

Remark : No information.
Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study
Species : rat
Sex : male/female
Strain : no data
Route of admin. : oral feed
Exposure period : at least 29 weeks per generation
Frequency of treatm. : Daily
Premating exposure period
Male : no data
Female : no data
Duration of test : no data
No. of generation studies : 3
Doses : 0.4%, 0.75% in diet
Control group : yes
NOAEL parental : = - .75 %
NOAEL F1 offspring : = - .75 %
NOAEL F2 offspring : = - .75 %
Result : No effect on reproduction
Method : other
Year : 1964
GLP : no
Test substance : other TS

Result : Diets containing either 0.40% or 0.75% phosphoric acid or 1.20% citric acid had no harmful effect on the growth of three successive generations of rats fed these diets.

There were no detrimental effect of the acid diets on reproduction either after the first or the second mating as judged by the weight of the mothers, the number of live young and stillborn young per litter, the average birth weight of the live young and the number of young left at weaning.

Test condition : Rats were fed a basal Dutch diet with average pH of 5.87 Three test groups received this diet to which either 0.4% or 0.75% phosphoric acid, or 1.2% citric acid were added.

A concentration of 0.5% phosphoric acid would provide, on the basis of body weight, the maximum acid intake in the human diet possible if the entire daily caloric requirements were obtained solely from the sugar present in phosphoric acid-containing soft drinks.

The average weights for each experimental group were measured at 0, 10 and 20 weeks after weaning. Reproduction of the rats in the test groups was investigated when they were 32 weeks old and had received the diets for 29 weeks. Eleven weeks later the same animals were mated again. Reproductive parameters measured were maternal bodyweight, number of live and stillborn young per litter, birth weight of live young and number of live young at weaning. However, no experimental detail of this reproductive study is included in the publication.

Test substance : Orthophosphoric Acid (CAS 7664-38-2). Batch and purity not stated,
Reliability : (4) not assignable
No experimental detail available for assessment of reliability.

04.07.2005 (25)

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	no data
Route of admin.	:	oral feed
Exposure period	:	no data
Frequency of treatm.	:	Daily
Premating exposure period		
Male	:	no data
Female	:	no data
Duration of test	:	no data
No. of generation studies	:	3
Doses	:	0.5% in diet
Control group	:	yes
NOAEL parental	:	= - .5 %
NOAEL F1 offspring	:	= - .5 %
NOAEL F2 offspring	:	= - .5 %
Result	:	No effect on reproduction
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	other TS

Remark : Reproductive section of published summary of an unpublished report: "Chronic oral toxicity studies of sodium tripolyphosphate in rats". Report dated 3 October 1959, carried out on behalf of Calgon Company by Professor Harold C Hodge and colleagues, Division of Pharmacology and Toxicology, University of Rochester School of Medicine and Dentistry, Rochester, New York.

Result : No effect on fertility or litter size, nor on growth or survival of offspring. Organ weights of third generation rats sacrificed at 1 month were unaffected. The macroscopic and microscopic appearance of major organs in third generation rats were comparable to controls.

Test condition : Reproduction studies covered three generations of rats reared and maintained on diets containing 0 and 0.5% sodium tripolyphosphate (TPP). Two litters were examined in each generation. Matings were carried out between 16 females and 8 males of each group when the rats were 100 days old.

Reproductive parameters measured were fertility, litter size, bodyweight, organ weights and survival of offspring. Macroscopic and microscopic appearance of main organs were examined in third-generation rats sacrificed at 1 month.

No detailed experimental procedure is given in the publication.

Test substance : Sodium trimetaphosphate, Curafos (TPP). Batch and purity not stated.

Reliability : (4) not assignable
Insufficient experimental detail is included in the publication for assessment of reliability.

04.07.2005 (26)

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	no data
Route of admin.	:	oral feed
Exposure period	:	no data
Frequency of treatm.	:	Daily
Premating exposure period		

Male	:	no data
Female	:	no data
Duration of test	:	no data
No. of generation studies	:	3
Doses	:	0.05% in diet
Control group	:	yes
NOAEL parental	:	= - .05 %
NOAEL F1 offspring	:	= - .05 %
NOAEL F2 offspring	:	= - .05 %
Result	:	No effect on reproduction
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	other TS
Remark	:	Reproductive section of published summary of an unpublished report: "Chronic oral toxicity studies of sodium trimetaphosphate in rats". Report dated 20 January 1960, carried out on behalf of Calgon Company by Professor Harold C Hodge and colleagues, Division of Pharmacology and Toxicology, University of Rochester School of Medicine and Dentistry, Rochester, New York.
Result	:	No effect on fertility or litter size, nor on growth or survival of offspring. Organ weights of third generation rats on weaning were unaffected. Histologically, tissues of third generation rats appeared normal.
Test condition	:	Reproduction studies covered three generations of rats reared and maintained on diets containing 0 and 0.05% sodium trimetaphosphate (TMP). Two litters were examined in each generation. Matings were carried out between 16 females and 8 males of each group when the rats were 100 days old. Reproductive parameters measured were fertility, litter size, bodyweight, organ weights and survival of offspring. Histological appearance of main organs were examined in third-generation rats sacrificed on weaning. No detailed experimental procedure is given in the publication.
Test substance	:	Sodium trimetaphosphate (TMP), batch number and purity not stated.
Reliability	:	(4) not assignable Insufficient experimental detail is included in the publication for assessment of reliability.

04.07.2005 (26)

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	no data
Route of admin.	:	oral feed
Exposure period	:	no data
Frequency of treatm.	:	Daily
Premating exposure period		
Male	:	no data
Female	:	no data
Duration of test	:	no data
No. of generation studies	:	3
Doses	:	0.5% in diet
Control group	:	yes
NOAEL parental	:	= - .5 %
NOAEL F1 offspring	:	= - .5 %
NOAEL F2 offspring	:	= - .5 %
Result	:	No effect on reproduction
Method	:	other

Year : 1964
GLP : no
Test substance : other TS

Remark : Reproductive section of published summary of an unpublished report: "Chronic oral toxicity studies of sodium hexametaphosphate in rats". Report dated 16 April 1960, carried out on behalf of Calgon Company by Professor Harold C Hodge and colleagues, Division of Pharmacology and Toxicology, University of Rochester School of Medicine and Dentistry, Rochester, New York.

Result : No effect on fertility or litter size, nor on growth or survival of offspring. In third generation rats, on abnormal organ weights or histological changes were evident.

Test condition : Reproduction studies covered three generations of rats reared and maintained on diets containing 0 and 0.5% sodium hexametaphosphate (HMP). Two litters were examined in each generation. Matings were carried out between 16 females and 8 males of each group when the rats were 100 days old.

Reproductive parameters measured were fertility, litter size, bodyweight, organ weights and survival of offspring. Histological appearance of main organs were examined in third-generation rats.

No detailed experimental procedure is given in the publication

Test substance : Sodium hexametaphosphate (Curafos URS, HMP), batch number and purity not stated.

Reliability : (4) not assignable
Insufficient experimental detail is included in the publication for assessment of reliability.

04.07.2005 (26)

Type : One generation study
Species : rat
Sex : no data
Strain : no data
Route of admin. : oral feed
Exposure period :
Frequency of treatm. : diets containing 0.75%(375mg/kgbw/d) no harmful effect
Premating exposure period
Male :
Female :
Duration of test : 29 wk
No. of generation studies :
Doses : 180-375mg/kgbw/d
Control group :

Remark : see ref (5)The higher dietary level of 0.75%PA (375mg/kgbw/d) apparently had no harmful effect on growth ofoffspring

Source : Grande Paroisse SA Paris la Defense 5
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994

Type : other
Species : Chinese hamster
Sex : no data
Strain : other
Route of admin. :
Exposure period :
Frequency of treatm. :
Premating exposure period

Male	:	
Female	:	
Duration of test	:	
No. of generation studies	:	
Doses	:	
Control group	:	
Remark	:	Effects of phosphoric acid on the growth, survival rate and macromolecular synthesis of mammalian cells of the Chinese hamster V79 lung cells that has been examined as themeasure of the product cytotoxicity. All effect appeared suddenly at or above 30mM in a short time.see ref (14)
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.02.1994 (27)

Type	:	other
Species	:	human
Sex	:	no data
Strain	:	
Route of admin.	:	
Exposure period	:	
Frequency of treatm.	:	
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	
No. of generation studies	:	
Doses	:	
Control group	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	no data
Remark	:	No information was located on the reproductive toxic potential of phosphoric acid or phosphates. see ref (5)
Source	:	Grande Paroisse SA Paris la Defense 5 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

04.07.2005

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	Gestation Days 6 through 15
Frequency of treatm.	:	Daily
Duration of test	:	Gestation Days 6 through 20
Doses	:	4.1, 19.0, 88.3, 410.0 mg/kg/day (bw)
Control group	:	yes
NOAEL maternal tox.	:	= 410 - mg/kg bw
NOAEL teratogen.	:	= 410 - mg/kg bw
Result	:	Not Teratogenic
Method	:	other
Year	:	1975
GLP	:	no

Test substance : other TS

Result : Mortality/Clinical Signs:
All rats survived the treatment and observation period. No clinical signs were recorded.

Bodyweight:
No effect on maternal bodyweight was reported in test animals.

Litter data:
There was no effect on number of corpora lutea, number of litters or average fetal weight and no clear effect on number of implantations or resorptions or litter size in any test group.

Teratological Effects:
The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring spontaneously in the sham-treated controls. In the positive control group, an increase in the number of resorptions and abnormalities in the nervous system (hydrocephalus, encephalomeningocoele, spina bifida) were reported.

The NOAEL for both maternal and fetal toxicity was 410 mg/kg bw.

Test condition : Virgin adult female albino rats (Wistar derived stock), 21 per group except for the high dose group with 20 animals, were mated with young adult males, and observation of the vaginal sperm plug was considered Day 0 of gestation. Beginning on Day 6 and continuing through Day 15 of gestation, the females were dosed with the test substance at doses of 4.1, 19.0, 88.3 or 410.0 mg/kg bw by oral intubation. The vehicle control group were dosed with water. The positive control group were dosed with aspirin at 250 mg/kg bw.

Dose (mg/kg/d)	Mated	Pregnant
0	21	20
Aspirin 250:	21	20
4.1	21	20
19	21	20
88.3	21	20
410.0	20	20

Body weights were recorded on Days 0, 6, 11, 15 and 20 of gestation. All animals were observed daily for appearance and behavior, with special attention given to food consumption and weight.

On Day 20, all dams were subjected to Caesarian Section. Sex, numbers of corpora lutea, implantation sites, resorption sites and live and dead fetuses were recorded. Body weights of live pups was recorded. The urinogenital tract of each dam was examined. All fetuses were examined grossly for external congenital abnormalities. One third of the fetuses of each litter underwent detailed visceral examination employing the Wilson technique. The remaining two thirds were cleared in potassium hydroxide, stained with alizarin red S dye and examined for skeletal defects.

Test substance : FDA 73-2: Anhydrous monosodium phosphate (CAS 7601-54-9), batch and purity not stated

Reliability : (2) valid with restrictions
Short study report, however the study meets generally accepted scientific principles, acceptable for assessment.

Flag : Critical study for SIDS endpoint
01.07.2005 (28)

Species : mouse
Sex : female
Strain : CD-1

Route of admin. : gavage
Exposure period : Gestation Days 6 through 15
Frequency of treatm. : Daily
Duration of test : Gestation Days 1 through 17
Doses : 3.7, 17.2, 79.7, 370.0 mg/kg/day bw
Control group : yes
NOAEL maternal tox. : = - 370 ml/kg bw
NOAEL teratogen. : = - 370 mg/kg bw
Result : Not teratogenic
Method : other
Year : 1975
GLP : no
Test substance : other TS

Result : Mortality/Clinical Signs:
All mice survived the treatment and observation period. No clinical signs were recorded.

Bodyweight:
No effect on maternal bodyweight was reported in test animals.

Litter data:
There was no effect on number of corpora lutea, number of litters or average fetal weight and no clear effect on number of implantations or resorptions or litter size in any test group.

Teratological Effects:
The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring spontaneously in the sham-treated controls.

The NOAEL for both maternal and fetal toxicity was 370.0 mg/kg bw.

Test condition : Virgin adult female albino CD-1 outbred mice were mated with young adult males, and observation of the vaginal sperm plug was considered Day 0 of gestation. Beginning on Day 6 and continuing through Day 15 of gestation, the females were dosed with the test substance at doses of 3.7, 17.2, 79.7 or 370.0 mg/kg bw by oral intubation. The vehicle control group were dosed with water. The positive control group were dosed with aspirin at 150 mg/kg bw. Numbers of animals used were:

Dose (mg/kg/d)	Mated	Pregnant
0	25	21
Aspirin 150:	27	20
3.7	25	22
17.2	25	19
79.7	25	20
370	25	22

All females were dosed, however only pregnant females were examined at term.

Body weights were recorded on Days 0, 6, 11, 15 and 17 of gestation. All animals were observed daily for appearance and behavior, with special attention given to food consumption and weight.

On Day 17, all dams were subjected to Caesarian Section. Sex, numbers of corpora lutea, implantation sites, resorption sites and live and dead fetuses were recorded. Body weights of live pups was recorded. The urinogenital tract of each dam was examined. All fetuses were examined grossly for external congenital abnormalities. One third of the fetuses of each litter underwent detailed visceral examination employing the Wilson technique. The remaining two thirds were cleared in potassium hydroxide,

stained with alizarin red S dye and examined for skeletal defects.

Test substance : FDA 73-2: Anhydrous monosodium phosphate (CAS 7601-54-9), batch and purity not stated

Reliability : (2) valid with restrictions
Short study report, however the study meets generally accepted scientific principles, acceptable for assessment.

Flag : Critical study for SIDS endpoint

29.06.2005 (28)

Species : rat
Sex : female
Strain : Wistar
Route of admin. : gavage
Exposure period : Gestation Days 6 through 15
Frequency of treatm. : Daily
Duration of test : Gestation Days 6 through 20
Doses : 2.82, 13.1, 60.7, 282.0 mg/kg/day bw
Control group : yes
NOAEL maternal tox. : = - 282 mg/kg bw
NOAEL teratogen. : = - 282 mg/kg bw
Result : Not teratogenic
Method : other
Year : 1975
GLP : no
Test substance : other TS

Result : Mortality/Clinical Signs:
All rats survived the treatment and observation period. No clinical signs were recorded.

Bodyweight:
No effect on maternal bodyweight was reported in test animals.

Litter data:
There was no effect on number of corpora lutea, number of implantations, number of litters, litter size or average fetal weight and no clear effect on resorptions in any test group.

Teratological Effects:
The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring spontaneously in the sham-treated controls. In the positive control group, an increase in the number of resorptions, skeletal and soft tissue abnormalities (encephalomeningocoele and gastroschisis) were reported.

The NOAEL for both maternal and fetal toxicity was 282 mg/kg bw.

Test condition : Virgin adult female albino rats (Wistar derived stock), 21 per group except for the high dose group with 20 animals, were mated with young adult males, and observation of the vaginal sperm plug was considered Day 0 of gestation. Beginning on Day 6 and continuing through Day 15 of gestation, the females were dosed with the test substance at doses of 2.82, 13.1, 60.7, 282.0 mg/kg bw by oral intubation. The vehicle control group were dosed with water. The positive control group were dosed with aspirin at 250 mg/kg bw.

Numbers of animals used were:

Dose (mg/kg/d)	Mated	Pregnant
0	28	25
Aspirin 250:	25	22
2.82	21	20
13.1	22	20
60.7	21	20

282.0 22 20

Body weights were recorded on Days 0, 6, 11, 15 and 20 of gestation. All animals were observed daily for appearance and behavior, with special attention given to food consumption and weight.

On Day 20, all dams were subjected to Caesarian Section. Sex, numbers of corpora lutea, implantation sites, resorption sites and live and dead fetuses were recorded. Body weights of live pups was recorded. The urinogenital tract of each dam was examined. All fetuses were examined grossly for external congenital abnormalities. One third of the fetuses of each litter underwent detailed visceral examination employing the Wilson technique. The remaining two thirds were cleared in potassium hydroxide, stained with alizarin red S dye and examined for skeletal defects.

Test substance : FDA 73-65: Anhydrous monopotassium phosphate (CAS 7778-53-2), batch and purity not stated

Reliability : (2) valid with restrictions
Short study report, however the study meets generally accepted scientific principles, acceptable for assessment.

Flag : Critical study for SIDS endpoint

01.07.2005 (29)

Species : mouse
Sex : female
Strain : CD-1
Route of admin. : gavage
Exposure period : Gestation Days 6 through 15
Frequency of treatm. :
Duration of test : Gestation Days 6 through 17
Doses : 3.2, 14.8, 68.9, 320.0 mg/kg/day bw
Control group : yes
NOAEL maternal tox. : = - 320 mg/kg bw
NOAEL teratogen. : = - 320 mg/kg bw
Result : Not teratogenic
Method : other
Year : 1975
GLP : no
Test substance : other TS

Result : Mortality/Clinical Signs:
All mice survived the treatment and observation period. No clinical signs were recorded.

Bodyweight:
No effect on maternal bodyweight was reported in test animals.

Litter data:
There was no effect on number of corpora lutea, litters or implantations, litter size or average fetal weight and no clear effect on number resorptions in any test group.

Teratological Effects:
The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring spontaneously in the sham-treated controls. In the positive control group, an increase in the number of resorptions, skeletal and soft tissue abnormalities (encephalomeningocoele and gastroschisis) were reported.

The NOAEL for both maternal and fetal toxicity was 410 mg/kg bw.

Test condition : Virgin adult female albino CD-1 outbred mice were mated with young adult males, and observation of the vaginal sperm plug was considered Day 0 of gestation. Beginning on Day 6 and continuing through Day 15 of gestation,

the females were dosed with the test substance at doses of 3.2, 14.8, 68.9 or 320.0 mg/kg bw by oral intubation. The vehicle control group were dosed with water. The positive control group were dosed with aspirin at 150 mg/kg bw.

Numbers of animals used were:

Dose (mg/kg/d)	Mated	Pregnant
0	23	22
Aspirin 150:	23	20
3.7	21	20
17.2	21	20
79.7	25	20
370	20	20

All females were dosed, however only pregnant females were examined at term.

Body weights were recorded on Days 0, 6, 11, 15 and 17 of gestation. All animals were observed daily for appearance and behavior, with special attention given to food consumption and weight.

On Day 17, all dams were subjected to Caesarian Section. Sex, numbers of corpora lutea, implantation sites, resorption sites and live and dead fetuses were recorded. Body weights of live pups was recorded. The urinogenital tract of each dam was examined. All fetuses were examined grossly for external congenital abnormalities. One third of the fetuses of each litter underwent detailed visceral examination employing the Wilson technique. The remaining two thirds were cleared in potassium hydroxide, stained with alizarin red S dye and examined for skeletal defects.

Test substance : FDA 73-65: Anhydrous monopotassium phosphate (CAS 7778-53-2), batch and purity not stated

Reliability : (2) valid with restrictions
Short study report, however the study meets generally accepted scientific principles, acceptable for assessment.

Flag : Critical study for SIDS endpoint

01.07.2005 (29)

Remark : No information.

Source : Leduc Chemie B.V. Amersfoort
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

16.12.1998

9. References

(1) ThermPhos International (1997): Produktinformation Phosphorsäure

(2) ThermPhos International (1997): Sicherheitsdatenblatt Phosphorsäure rein 85 %

(3) Hoechst AG (1991): Produktinformation Phosphorsaeure der Abt. Marketing Chemikalien (Februar 1991)

(4) Hoechst AG (1994): Sicherheitsdatenblatt Phosphorsaeure rein 85 prozentig (27.04.1994)

(5) US-EPA (1990): Fed. Regist. 55(122), 25876-25878 (25.06.1990)

(6) boiling point > 135°C at atmospheric pressure for a 75% solution as given by BASF Sicherheitsdatenblatt Phosphorsaeure.

(7) BASF AG, Sicherheitsdatenblatt Phosphorsaeure (12/90). Bezieht sich auf 75 %ige H3PO4.

(8) BASF Sicherheitsblatt Phosphorsaeure 75% solution

(9) BASF sicherheitsblatt Phosphorsaeure 75% solution

(10) Hoechst AG (1992): Interne Mitteilung der Abt. F+E Chemikalien (09.09.1992)

(11) (4) Ellgaard,E.G. Gilmore,J.Y.Jr. 1984, J. Fish Biol. 25 (2)133-7, see also ref (2)

(12) Ellgaard, Gilmore (1984): J. Fish Biol. 25(2), 133-137

(13) (5) Phosphoric acid/phosphates a Review, Von Burg, R.,J. Appl. Tox. 12, (4), 301-3, 1992.

(14) (6) Brehm, Meijerling, Arch Hydrobiol 95, (1-4) 17-27, 1982

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(16) BIOFAX Ind. (1970): Bio-Test Lab. 17-4/70; zitiert in: RTECS (1991)

(17) see ref (1)

(18) HSDB AN 001187 (Hazardous Substance Data Bank)

(19) SAX: Dangerous properties of industrial Material

(20) see ref (2) and also Dangerous properties of industrial Materials, Sax.

(21) (11) Acute toxic evaluation of various concentrations of phosphoric acid, Randall,D.J., Robinson, E.C., Acute toxic. data, 1 (1), 69-70, 1990

(22) see ref (1) and ref (3)p.55

(23) (13) Al Ani,F.Y., Al Lami, S.K., Absence of mutagenic activity of acidity regulators in the Ames/samonella test, Mutat. Res., 206, (4), 467-70, 1988.

(24) (13) Sublethal pH decrease may cause genetic damage to eucaryotic cell: a study on sea urchins and S. typhimurium, Cipollaro, M. Corsale, G. et al, Terato, carcio, mutagenesis6, 275-87, 1986

(25) Bonting SL, Jansen BCP (1956), "The effect of a prolonged intake of phosphoric acid and citric acid in rats", Netherlands J Nutrition, 17: 137-148 (published)

(26) BIBRA (1964), "Summaries of Toxicological Data: Toxicity Studies on Phosphates:", Fd Cosmet Toxicol. 2:147-154 (published

(27) (14) Cytotoxicity of phosphoric acid on cultured mammalian cells, Iijima, Horii, Kanemaki et al, Shigaku, 80, (5) 1159-65, 1993

(28) NTIS (1975), "Teratological Evaluation of FDA 73-2, Monosodium Phosphate, Anhydrous in Mice and Rats", Food and Drugs Research Labs., Inc., Waverley, N.Y. (published)

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IUCLID Dataset

Existing Chemical	Substance ID: 149-57-5
CAS No.	149-57-5
EINECS Name	2-ethylhexanoic acid
EINECS No.	205-743-6
Molecular Formula	C8H16O2

Dataset created by: EUROPEAN COMMISSION - European Chemicals Bureau

This dossier is a compilation based on data reported by the European Chemicals Industry following 'Council Regulation (EEC) No. 793/93 on the Evaluation and Control of the Risks of Existing Substances'. All (non-confidential) information from the single datasets, submitted in the IUCLID/HEDSET format by individual companies, was integrated to create this document.

The data have not undergone any evaluation by the European Commission.

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European Chemicals Bureau

1.0.1 OECD and Company Information

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Street: Industriepark Höchst
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Country: Germany

Name: Eastman Chemical B.V.
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Town: 65903 Frankfurt/Main
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Name: Huels AG
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Town: D-45764 Marl
Country: Germany

Name: Lagor S.p.A.
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Town: 21013 Gallarate
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Name: Neste Oxo AB
Town: 44484 Stenungsund
Country: Sweden
Phone: +46 303 85600
Telefax: +46 303 856 07
Telex: 27052 nestox S

1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

-

1.1 General Substance Information

Substance type: organic
Physical status: liquid

1.1.1 Spectra

-

1.2 Synonyms

"EASTMAN" 2-ethylhexanoic acid
Source: Eastman Chemical B.V. The Hague

.alpha.-Ethylcaproic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

.alpha.-Ethylhexanoic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

2-Butylbutanoic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

2-Ethyl-1-hexanoic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

2-Ethylcaproic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

2-Ethylcapronsaeure
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-ethylhexanoic acid
Source: Eastman Chemical B.V. The Hague

2-Ethylhexanoic acid
Source: BASF AG Ludwigshafen
Hoechst AG Frankfurt/Main
Huels AG Marl
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexansaeure
Source: BASF AG Ludwigshafen
Hoechst AG Frankfurt/Main
Huels AG Marl
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexoic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

3-Heptanecarboxylic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

Acido 2etil esoico
Source: Lagor S.p.A. Gallarate

Alpha-Ethylhexansaeure
Source: BASF AG Ludwigshafen
Huels AG Marl

alpha-Ethylhexansaeure
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Butylethylacetic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

Ethylhexanoic acid
Source: BASF AG Ludwigshafen
Huels AG Marl

Hexanoic acid, 2-ethyl- (8CI, 9CI)
Source: BASF AG Ludwigshafen
Huels AG Marl

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

Quantity 100 000 - 500 000 tonnes

1.6.1 Labelling

Labelling: as in Directive 67/548/EEC
Symbols: Xn
D
Specific limits: no data
R-Phrases: (63) Possible risk of harm to the unborn child
S-Phrases: (2) Keep out of reach of children
(36/37) Wear suitable protective clothing and gloves

1.6.2 Classification

Classification: as in Directive 67/548/EEC
Class of danger: toxic for reproduction, category 3
R-Phrases: (63) Possible risk of harm to the unborn child

1.7 Use Pattern

Type: type
Category: Non dispersive use

Type: type
Category: Use in closed system

Type: type
Category: Use resulting in inclusion into or onto matrix

Type: industrial
Category: Chemical industry: used in synthesis

Type: use
Category: Intermediates

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

Type of limit: MAK (DE)
Limit value:
Remark: kein MAK-Wert festgelegt
Source: BASF AG Ludwigshafen

(1)

Type of limit: MAK (DE)
Limit value:
Country: Germany
Remark: MAK not established
Source: Huels AG Marl

(2)

Type of limit:
Limit value:
Remark: No threshold limits have been established.
Source: Eastman Chemical B.V. The Hague

Type of limit:
Limit value:
Remark: Non stabilito.
Source: Lagor S.p.A. Gallarate

1.9 Source of Exposure

Memo: Emissionserklaerung Huels 1992
Remark: Release into the atmosphere on production site in 1992: less than 25 kg/a
Source: Huels AG Marl

(3)

Remark: La sostanza è utilizzata per usi esclusivamente industriali ed è manipolata solo da operatori addestrati. La manipolazione è minima.
Source: Lagor S.p.A. Gallarate

1.10.1 Recommendations/Precautionary Measures

-

1.10.2 Emergency Measures

-

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

Classified by: KBwS (DE)
Labelled by:
Class of danger: 1 (weakly water polluting)
Source: BASF AG Ludwigshafen

Classified by: KBwS (DE)
Labelled by:
Class of danger: 1 (weakly water polluting)
Remark: Kenn-Nr. 1179 (Wassergefährdungsklasse - WGK)
Source: Hoechst AG Frankfurt/Main

(4) (5) (6)

Classified by: KBwS (DE)
Labelled by:
Class of danger: 1 (weakly water polluting)
Remark: Kenn-Nr. 1179 (Wassergefährdungsklasse - WGK)
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(4)

Classified by: other: BASF
Labelled by: other: BASF
Class of danger: 1 (weakly water polluting)
Source: BASF AG Ludwigshafen

Classified by: other: Huels AG
Labelled by: other: Huels AG
Class of danger: 1 (weakly water polluting)
Country: Germany
Source: Huels AG Marl

(2)

1.14.2 Major Accident Hazards

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Source: BASF AG Ludwigshafen

(7)

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Source: Hoechst AG Frankfurt/Main

(5)

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Country: Germany
Remark: Stoerfallverordnung 1991
Source: Huels AG Marl

(2)

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(8)

1.14.3 Air Pollution

Classified by: TA-Luft (DE)
Labelled by:
Number: 3.1.7 (organic substances)
Class of danger: III
Remark: Selbsteinstufung
Source: Hoechst AG Frankfurt/Main

(9) (5) (6)

Classified by: TA-Luft (DE)
Labelled by:
Number: 3.1.7 (organic substances)
Class of danger: III
Remark: Selbsteinstufung
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(8) (9) (6)

1.15 Additional Remarks

Remark: La sostanza può essere eliminata mediante incenerimento in condizioni controllate con abbattimento dei fumi, secondo lenorme vigenti.
Merce non pericolosa ai fini del trasporto, secondo le normevigenti.
Source: Lagor S.p.A. Gallarate

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2.1 Melting Point

Value: < -60 degree C
Source: BASF AG Ludwigshafen
(10) (11)

Value: < -60 degree C
Source: Hoechst AG Frankfurt/Main
(5)

Value: < -60 degree C
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

Value: ca. -59 degree C
Source: BASF AG Ludwigshafen
(12)

2.2 Boiling Point

Value: ca. 226 - 229 degree C at 1013 hPa
Method: other: DIN 51 751
Source: BASF AG Ludwigshafen
(12)

Value: = 227.5 degree C at 1013 hPa
Source: BASF AG Ludwigshafen
(10)

Value: = 228 degree C at 1013 hPa
Source: BASF AG Ludwigshafen
(11)

Value: = 228 degree C at 1013 hPa
Source: Hoechst AG Frankfurt/Main
(5)

Value: = 228 degree C at 1013 hPa
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

2.3 Density

Type: density
Value: .905 - .907 g/cm3 at 20 degree C
Method: other: DIN 51757, Verfahren D
Source: BASF AG Ludwigshafen
(10)

Type: density
Value: = .906 g/cm3 at 20 degree C
Method: other: DIN 51757
Source: BASF AG Ludwigshafen
(11)

Type: density
Value: = .906 g/cm3 at 20 degree C
Method: other: DIN 51757
Source: Hoechst AG Frankfurt/Main
(5)

Type: density
Value: = .906 g/cm3 at 20 degree C
Method: other: DIN 51757
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

Type: density
Value: = .91 g/cm3 at 20 degree C
Remark: DIN 51 757
Source: BASF AG Ludwigshafen
(12)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: = .04 hPa at 20 degree C
Source: BASF AG Ludwigshafen
(12)

Value: < .1 hPa at 20 degree C
Source: BASF AG Ludwigshafen
(11)

Value: < .1 hPa at 20 degree C
Source: Hoechst AG Frankfurt/Main
(5)

Value: < .1 hPa at 20 degree C
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

Value: ca. .3 hPa at 50 degree C
Source: Hoechst AG Frankfurt/Main
(5)

Value: ca. .3 hPa at 50 degree C
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

2.5 Partition Coefficient

log Pow: = 2.64
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year:
Source: BASF AG Ludwigshafen

log Pow: = 2.64
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year:
Source: Hoechst AG Frankfurt/Main
(5)

log Pow: = 2.64
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year:
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

log Pow: = 2.7
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year:
Source: BASF AG Ludwigshafen
(13)

log Pow: = 2.81
Method: other (calculated): Inkrementenmethode von Rekker
Year:
Source: BASF AG Ludwigshafen
(14)

2.6.1 Water Solubility

Value: = .2 at 20 degree C
Qualitative: slightly soluble
Remark: Wert: =0.2 sonstige: %(m/m) bei 20 Grad C
Source: BASF AG Ludwigshafen
(10)

Value: = 1.4 g/l at 20 degree C
pH: ca. 3 at 1.4 g/l and 20 degree C
Source: BASF AG Ludwigshafen
(12)

Value: = 2 g/l at 20 degree C
pH: ca. 3.3 at 2 g/l and 20 degree C
Source: BASF AG Ludwigshafen
(11)

Value: = 2 g/l at 20 degree C
pH: ca. 3.3 at 2 g/l and 20 degree C
Source: Hoechst AG Frankfurt/Main
(5)

Value: = 2 g/l at 20 degree C
pH: ca. 3.3 at 2 g/l and 20 degree C
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

2.6.2 Surface Tension

-

2.7 Flash Point

Value: ca. 114 degree C
Type: closed cup
Method: other: DIN 51758
Year:
Source: BASF AG Ludwigshafen
(12) (15) (11)

Value: = 114 degree C
Type: closed cup
Method: other: DIN 51758
Year:
Source: Hoechst AG Frankfurt/Main
(5) (6)

Value: = 114 degree C
Type: closed cup
Method: other: DIN 51758 / DIN EN 22719 / ISO 2719
Year:
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8) (6)

2.8 Auto Flammability

Value: = 320 degree C
Method: other: DIN 51794
Remark: Zuendtemperatur
Source: Hoechst AG Frankfurt/Main
(5) (6)

Value: = 320 degree C
Method: other: DIN 51794
Remark: Zuendtemperatur
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8) (6)

Value:
Remark: Zuendtemperatur: 310 Grad C (DIN 51 794)
Source: BASF AG Ludwigshafen
(16)

Value:
Remark: Zuendtemperatur: = 320 Grad C
Methode: DIN 51794
Source: BASF AG Ludwigshafen
(10) (11)

Value:
Remark: Zuendtemperatur: = 320 Grad C
Methode: DIN 51794
Source: BASF AG Ludwigshafen
(10) (11)

2.9 Flammability

-

2.10 Explosive Properties

Result: other
Remark: Untere Explosionsgrenze: 1.2 Vol-%
Source: Hoechst AG Frankfurt/Main
(5)

Result: other
Remark: Untere Explosionsgrenze: 1.2 Vol-%
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

Result:
Remark: Explosionsgrenzen in Luft: 0.9 - 6.7 Vol. %
Source: BASF AG Ludwigshafen
(12)

Result:
Remark: Untere Explosionsgrenze: 1.2 Vol.%
Gefaehrliche Reaktionen mit Alkalien (Laugen).
Source: BASF AG Ludwigshafen
(11)

Result:
Remark: Untere Explosionsgrenze: 1.2 Vol.%
Gefaehrliche Reaktionen mit Alkalien (Laugen).
Source: BASF AG Ludwigshafen
(11)

2.11 Oxidizing Properties

-

2.12 Additional Remarks

Remark: Gefaehrliche Reaktionen: exotherme Reaktion mit Basen.
Source: BASF AG Ludwigshafen
(12)

Remark: Viskositaet bei 20 Grad C: 7.7 mPas (Methode: DIN 51562).
Mit den gebraeuchlichen organischen Loesemitteln mischbar.
Source: BASF AG Ludwigshafen
(10)

Remark: Viskositaet bei 20 Grad C: 7.7 mPas (Methode: DIN 51562).
Mit den gebraeuchlichen organischen Loesemitteln mischbar.
Source: BASF AG Ludwigshafen
(10)

Remark: Viskositaet bei 20 Grad C: 7.7 mPa*s (Methode: DIN 51562)
Mit den gebraeuchlichen organischen Loesemitteln mischbar.
Source: Hoechst AG Frankfurt/Main
(6)

Remark: Gefaehrliche Reaktionen: Mit Alkalien (Laugen)
Source: Hoechst AG Frankfurt/Main
(5)

Remark: Viskositaet bei 20 Grad C: 7.7 mPa*s (Methode: DIN 51562)
Mit den gebraeuchlichen organischen Loesemitteln mischbar.
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(6)

Remark: Gefaehrliche Reaktionen: Mit Alkalien (Laugen)
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(8)

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .000000000008037 cm3/(molecule * sec)
Degradation: ca. 50 % after 16 hour(s)
Method: other (calculated): ATMOSPHERIC OXIDATION PROGRAMM, Version 1.51 vom 13.03.94,Syracuse Research Corporation, nach Atkinson (1987 und 1988)
Year: **GLP:**
Test substance:
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(17)

Type: other
Method:
Year: **GLP:**
Test substance:
Remark: K=8.04E-12 cm3/mol*s; berechnet mit AOP nach Meylan
Source: BASF AG Ludwigshafen

(18)

3.1.2 Stability in Water

Type:
Method: other
Year: **GLP:**
Test substance:
Remark: no data available
Source: BASF AG Ludwigshafen

3.1.3 Stability in Soil

Type: **Radiolabel:**
Concentration:
Cation exch. capac.
Microbial biomass:
Method: other: estimated value
Year: **GLP:**
Test substance:
Remark: Anhand der Regressionsgleichung (log Koc = 0.544 log Pow + 1.377) wurde ueber den log Pow ein Bodensorptionskoeffizient Koc von 701.13 bestimmt.
Source: BASF AG Ludwigshafen

(19)

3.2 Monitoring Data (Environment)

Type of measurement: other: GC-MS
Medium:
Remark: 2-Ethylhexansaeure wurde in der Luft entlang des Niagara River waehrend eines Feldversuches in der Zeit vom 14-21 Sept. 1982 qualitativ mittels "reconstructed ion chromatograms" (RICs) identifiziert.
Source: BASF AG Ludwigshafen

(20)

3.3.1 Transport between Environmental Compartments

Type: volatility
Media: water - air
Method: other: estimated value
Year:
Remark: Mit einer Wasserloeslichkeit von S=9.7 mol/m^3 und einem Dampfdruck von p=0.04 hPa ergibt die Berechnung nach H=p/S eine Henry-Konstante von 0.0041237 hPa*m^3/mol fuer die Saure.
Source: BASF AG Ludwigshafen

(19)

3.3.2 Distribution

Media: other
Method:
Year:
Remark: no data available
Source: BASF AG Ludwigshafen

3.4 Mode of Degradation in Actual Use

Remark: no data are available
Source: BASF AG Ludwigshafen

3.5 Biodegradation

Type: aerobic
Inoculum: other: BASF-Belebtschlamm
Degradation: = 39 % after 28 day
Result: other: im Sinne der EG-Richtlinie nicht leicht abbaubar
Method: other: EEC Directive 79-831, Annex V; Determination of the "ready biodegradability"; Part IV, Manometric Respirometry
Year: 1991 **GLP:** no
Test substance: other TS
Remark: Dieser Test ist aufgrund der Pruefsubstanz fuer die Kennzeichnung von 2-Ethylhexansaeure nicht relevant.
Source: BASF AG Ludwigshafen
Test substance: 2-Ethylhexansaeurechlorid-Rueckstand (wasserunloesliche Anteile)

(21)

Type: aerobic
Inoculum: activated sludge
Degradation: = 39 % after 28 day
Result: other: im Sinne der EG-Richtlinie nicht leicht abbaubar
Method: other: EEC Directive 79-831, Annex V;Methods for the Determination of Ecotoxicity;CY.
Year: **GLP:** no
Test substance:
Source: BASF AG Ludwigshafen
Test condition: Es wurde 2-Ethylhexansaeurechlorid geprueft.

(22)

Type: aerobic
Inoculum: activated sludge
Degradation: > 95 % after 5 day
Method: other: Standversuch (CSB)
Year: **GLP:** no
Test substance:
Remark: Elimination durch nichtbiologische Vorgaenge kleiner 10%, biologisch leicht abbaubar.
Sekundaerzitat
Source: BASF AG Ludwigshafen

(23)

Type: aerobic
Inoculum: activated sludge
Degradation: = 100 % after 3 day
Method: other: Standversuch; (TOD)
Year: **GLP:**
Test substance:
Remark: Gut eliminierbar, biologisch abbaubar.
Source: BASF AG Ludwigshafen

(24)

Type: aerobic
Inoculum: activated sludge, industrial
Degradation: > 95 % after 5 day
Method: other: Zahn-Wellens-Test nach den Richtlinien von 1979
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: CSB-Eliminierung durch nichtbiologische Vorgaenge: < 10 %
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(25)

Type: anaerobic
Inoculum:
Method:
Year: **GLP:**
Test substance:
Remark: A 20-litre anaerobic biofilter, packed with expanded clay pellets, was used to treat 2-ethylhexanoic acid. The biofilter was operated for 425 days, at decreasing hydraulic retention times (HRT) from 20 to 0.83 days, with an influent 2-ethylhexanoic acid concentration of 8200 mg/l. COD removal efficiency was 92.8 %, and the biogas production rate aver-aged 128.7 l/day with 83.0 % of methane. The pH of the bio-filter liquor remained between 6.9 and 7.5, right up to the time when the biofilter finally failed at 0.83 day HRT. At that point of failure, the COD removal efficiency was 20.1 %. Failure resulted in the accumulation of 2-ethyl-hexanoic acid in the reactor liquor, which averaged 4407 mg/l.
Source: BASF AG Ludwigshafen

(26)

3.6 BOD5, COD or BOD5/COD Ratio

C O D

Method: other: DIN 38409 Teil 41/1
COD: = 2113 mg/g substance

Remark: BSB = 823 mg/g after 28 days
Die CSB-Bestimmung bei schwer wasserloeslichen Substanzen ist nicht immer zuverlaessig durchfuehrbar.
Source: BASF AG Ludwigshafen
Test condition: Geprueft wurde 2-Ethylhexansaeurechlorid.

(22)

C O D

Method: other: DIN 38409 Teil 41/1
Year: 1991 **GLP:** no
COD: = 2113 mg/g substance

Remark: BSB = 823 mg/g
Die CSB-Bestimmung bei schwer wasserloeslichen Substanzen ist nicht immer zuverlaessig durchfuehrbar.
Dieser Test ist aufgrund der Pruefsubstanz fuer die Kennzeichnung von 2-Ethylhexansaeure nicht relevant.
Source: BASF AG Ludwigshafen
Test substance: 2-Ethylhexansaeurechlorid-Rueckstand (wasserunloesliche Anteile)

(21)

3.7 Bioaccumulation

Species:
Exposure period:
Concentration:
BCF:
Elimination:
Method: other: estimated value
Year: **GLP:**
Test substance:
Remark: Based on a measured log Pow of 2.7, (for free acid) the bioconcentration factor (BCF) for 2-ethylhexanoic acid can be estimated to be 66.37 from a recommended regression-derived equation (log BCF = 0.76*log Pow - 0.23)
Source: BASF AG Ludwigshafen

(27)

3.8 Additional Remarks

-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: other: force feeding
Species: Cyprinus carpio (Fish, fresh water)
Exposure period:
Unit: **Analytical monitoring:** no
NOEL : >= 117
Method: other: dose levels of 88, 109 or 117 mg/kg bodyweight were force fed to carps
Year: **GLP:** no data
Test substance: other TS
Result: No treatment related effects were observed.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(28)

Type: static
Species: Lepomis gibbosus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 160
LC50: = 270
LC100: = 400
Method: other: keine Angaben
Year: 1979 **GLP:** no
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: Substanz chemisch rein

(29)

Type: static
Species: Lepomis gibbosus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 160
LC50: = 270
LC100: = 400
Method: other: keine Angaben
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(30)

Type: static
Species: Lepomis gibbosus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 160
LC50: = 270
LC100: = 400
Method: other: keine Angaben
Year: 1979 **GLP:** no
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: Substanz chemisch rein

(31)

Type: static
Species: Lepomis gibbosus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 160
LC50: = 270
LC100: = 400
Method: other: keine Angaben
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(30)

Type: static
Species: Leuciscus idus melanotus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
SG : = 250
Method: other: DIN 38412
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: SG = Schaedlichkeitsgrenze
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(25)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 125
LC50: = 180
LC100: = 250
Method: other: keine Angaben
Year: 1979 **GLP:** no
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: Substanz chemisch rein

(32)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 125
LC50: = 180
LC100: = 250
Method: other: keine Angaben
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(33)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 125
LC50: = 180
LC100: = 250
Method: other: keine Angaben
Year: 1979 **GLP:** no
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: Substanz chemisch rein

(32)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 125
LC50: = 180
LC100: = 250
Method: other: keine Angaben
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(33)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:**
EC0: = 62.5
EC50: = 116.6
EC100: = 250
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:**
EC0: = 62.5
EC50: = 85.4
EC100: = 125
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(34)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint:
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:**
EC10: = 33
EC50: = 61
Method: other: Scenedesmus-Zellvermehrungs-Hemmtest, DIN 38412 Teil 9, Bestimmung der Hemmwirkung von Wasserinhaltsstoffen auf Gruenalgen
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(35)

Species: Scenedesmus subspicatus (Algae)
Endpoint:
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:**
EC10: = 25
EC50: = 41
Method: other: Scenedesmus-Zellvermehrungs-Hemmtest, DIN 38412 Teil 9, Bestimmung der Hemmwirkung von Wasserinhaltsstoffen auf Gruenalgen
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(35)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 30 minute(s)
Unit: mg/l **Analytical monitoring:**
EC20 : = 650
Method: OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year: 1984 **GLP:**
Test substance:
Remark: Geprueft wurde 2-Ethylhexansaeurechlorid.
Da der Stoff wasserunloeslich ist, wurden 2000 mg in 500 ml Ethanol geloest und so als Stammloesung im Test eingesetzt.
Hoechste getestete Konzentration betrug 1003 mg/l.
Source: BASF AG Ludwigshafen

(22)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 30 minute(s)
Unit: mg/l **Analytical monitoring:**
EC10: = 250
EC50: = 670
EC90 : = 930
Method: other: Pseudomonas-Atmungs-Hemmtest, DIN 38412 Teil 27, in Vorber., Bestimmung der Hemmwirkung von Abwasser auf die Sauerstoffzehrung von Pseudomonas putida
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(34)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 17 hour(s)
Unit: mg/l **Analytical monitoring:**
EC10: = 72
EC50: = 110
EC90 : = 220
Method: other: Pseudomonas-Zellvermehrungs-Hemmtest, DIN 38412 Teil 8, zum Gelbdruck verabschiedet, Bestimmung der Hemmwirkung von Wasserinhaltsstoffen auf Bakterien
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(34)

Type: aquatic
Species: other bacteria: BASF-Belebtschlamm
Exposure period: 30 minute(s)
Unit: mg/l **Analytical monitoring:**
EC20 : = 650
Method: OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year: 1991 **GLP:** no
Test substance: other TS
Remark: Geprueft wurde 2-Ethylhexansaeurechlorid-Rueckstand (wasser-unloesliche Bestandteile).
Da der Stoff wasserunloeslich ist, wurden 2000 mg in 500 ml Ethanol geloest und so als Stammloesung im Test eingesetzt.
Hoechste getestete Konzentration betrug 1003 mg/l.
Source: BASF AG Ludwigshafen

(21)

Type: aquatic
Species: anaerobic bact. from a domestic water treatment plant
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
SG : = 600
Method: ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: SG = Schaedlichkeitsgrenze
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(25)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: other
Endpoint:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: no data available
Source: BASF AG Ludwigshafen

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type: other
Species:
Endpoint:
Exposure period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: no data available
Source: BASF AG Ludwigshafen

4.6.2 Toxicity to Terrestrial Plants

Species:
Endpoint:
Expos. period:
Unit:
Method: other
Year: **GLP:**
Test substance:
Remark: no data available
Source: BASF AG Ludwigshafen

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

Species: other
Endpoint:
Expos. period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: no data available
Source: BASF AG Ludwigshafen

4.7 Biological Effects Monitoring

Remark: no data available
Source: BASF AG Ludwigshafen

4.8 Biotransformation and Kinetics

Type: other
Remark: no data available
Source: BASF AG Ludwigshafen

4.9 Additional Remarks

-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 3000 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(36)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 3000 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(37)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 3640 mg/kg bw
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(38) (39)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 3276 mg/kg bw
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(40)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 2043 mg/kg bw
Method:
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: LD50 fuer weibl. F344 Ratten;
Applikationsform: Schlundsonde
Source: BASF AG Ludwigshafen
(41) (42) (43)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 3000 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen
(37)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: ca. 2000 - 3000 mg/kg bw
Method: other: no details reported
Year: **GLP:** no data
Test substance: other TS
Remark: At 720 mg/kg no mortality occurred. No further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.
(44)

Type:
Species: rat
Sex:
Number of Animals:
Vehicle:
Value:
Method:
Year: **GLP:**
Test substance:
Remark: 3200 mg/kg 2-Ethylhexansaeure wirkten bei Ratten letal; die Tiere, die 1600 mg/kg bekamen ueberlebten.
Source: BASF AG Ludwigshafen

(45) (46) (47)

Type:
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value:
Method:
Year: **GLP:**
Test substance:
Remark: 1600 mg/kg oral an Meerschweinchen appliziert wirkten letal, die Tiere die 800 mg/kg erhielten ueberlebten.
Source: BASF AG Ludwigshafen

(45) (46) (47)

Type:
Species:
Sex:
Number of Animals:
Vehicle:
Value:
Method:
Year: **GLP:**
Test substance:
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5.1.2 Acute Inhalation Toxicity

Type: LC0
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value: = 2.36 mg/l
Method: other: 3 rats were exposed and observed for 14 days
Year: **GLP:** no data
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(48)

Type: LC50
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value: > .015 mg/l
Method:
Year: **GLP:**
Test substance:
Remark: Waehrend und nach 6-stuendiger Exposition von Ratten gegenueber 0.015 mg/l 2-Ethylhexansaeure konnten bei den Tieren keine Symptome festgestellt werden.
Source: BASF AG Ludwigshafen

(45) (46) (47)

Type: other: IRT
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 8 hour(s)
Value:
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: Keine Mortalitaet nach 8 Stunden Exposition in einer bei 20 Grad Celsius angereicherten bzw. gesaettigten Atmosphaere.
Source: BASF AG Ludwigshafen

(38) (39)

Type: LC50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value: > 2.39 mg/l
Method: other: no details reported, 400 ppm are given as concentration
Year: **GLP:** no data
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(49)

Type: other: IRT
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Exposure time: 8 hour(s)
Value:
Method:
Year: **GLP:**
Test substance:
Remark: Keine Mortalitaet nach 8 Stunden Exposition in einer bei 20 Grad Celsius angereicherten bzw. gesaettigten Atmosphaere.
Source: BASF AG Ludwigshafen

(50)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 2000 mg/kg bw
Method: OECD Guide-line 402 "Acute dermal Toxicity"
Year: 1986 **GLP:** yes
Test substance: other TS
Remark: Stamm: Wistar, maennlich weiblich
Source: BASF AG Ludwigshafen
Test substance: Substanzreinheit >99%

(51)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 2000 mg/kg bw
Method: OECD Guide-line 402 "Acute dermal Toxicity"
Year: 1986 **GLP:** yes
Test substance: other TS
Remark: Stamm: Wistar, männlich und weiblich
Source: Hoechst AG Frankfurt/Main
Test substance: Substanzreinheit > 99 %

(52)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 2000 mg/kg bw
Method: OECD Guide-line 402 "Acute dermal Toxicity"
Year: 1986 **GLP:** yes
Test substance: other TS
Remark: Stamm: Wistar, männlich und weiblich
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test substance: Substanzreinheit > 99 %

(52)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: 1260 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(36)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: 5700 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(39)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: 6300 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen
(37)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: 5690 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen
(46)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: ca. 6500 mg/kg bw
Method: other: 6 animals were used, occlusive application for 4 days, observation for 14 days
Year: **GLP:** no data
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.
(53)

Type: other: lethal dose
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: <= 5000 - 10000 mg/kg bw
Method: other: only single animals were used per dose, all animals died
Year: **GLP:** no data
Test substance: other TS
Remark: The substance was applied occluded for 24 hours. No further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.
(54)

Type:
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: 4550 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Remark: Die 24 stuendige okklusive Applikation von 5 ml/kg (4550 mg/kg) auf der Haut von Meerschweinchen fuehrte zum Tod der Tiere. Die Hautreizwirkung wurde als leicht reizend bezeichnet.
Source: BASF AG Ludwigshafen

(45) (47)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: 270 mg/kg bw
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(38)

Type:
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: 1600 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Remark: Die i.p. Applikation von 1600 mg/kg 2-Ethylhexansaeure wirkte bei Ratten letal.
Source: BASF AG Ludwigshafen

(47)

Type:
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: 400 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Remark: Die i.p. Applikation von 400 mg/kg 2-Ethylhexansaeure wirkte bei Meerschweinchen letal.
Source: BASF AG Ludwigshafen

(47)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: s.c.
Value: 910 mg/kg bw
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(40)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method:
Year: **GLP:**
Test substance:
Remark: Die Reizwirkung wurde von den Autoren mit leicht angegeben.
Source: BASF AG Ludwigshafen

(55)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: corrosive
EC classificat.:
Method: other: 4 Stunden okklusiv
Year: **GLP:**
Test substance:
Remark: Bei 2 von 4 Tieren wurde Nekrosenbildung beschrieben. Die Autoren bezeichneten 2-Ethylhexansaeure als "corrosive material".
Source: BASF AG Ludwigshafen

(56)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: slightly irritating
EC classificat.:
Method: other: Smyth Carpenter
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(57)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(38) (58)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: 20 Std. Applikation
Source: BASF AG Ludwigshafen

(40)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.: not irritating
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(59)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other: Smyth Carpenter
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(57)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.: not irritating
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1981 **GLP:** yes
Test substance: other TS
Source: BASF AG Ludwigshafen

(59)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: corrosive
EC classificat.:
Method: other: 6 rabbits were used, occlusive application for 4 hours, evaluation at 4 and 48 hours
Year: **GLP:** no data
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: 2-Ethylhexanoic Acid, no further data.

(60)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other: no details reported
Year: **GLP:** no data
Test substance: other TS
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(61)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: corrosive
EC classificat.:
Method: other: US Department of Transportation Corrosivity Test
Year: **GLP:** yes
Test substance: other TS
Remark: The test material produced slight necrosis in 5 of 6 animalsafter 4 hours with subsequent eschar formation (slight to moderate), no further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(62)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.: not irritating
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1985 **GLP:** yes
Test substance: other TS
Remark: Stamm: Neuseeländer
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test substance: Substanzreinheit 99 %

(63)

Species: guinea pig
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: corrosive
EC classificat.:
Method: other: 2 animals/group were used, exposure was occluded for 24 hours.
Year: **GLP:** no
Test substance: other TS
Remark: The effects are described by the reviewer as slight edema, erythema and necrosis, no further details are reported.
Source: BASF AG Ludwigshafen

Test substance: 2-ethylhexanoic acid, no further data.

(54)

Species: rat
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other: 24; 48; 72 oder 96 Std. okklusiv
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(42) (43)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method:
Year: **GLP:**
Test substance:
Remark: Die Wirkung wurde mit stark reizend angegeben.
Source: BASF AG Ludwigshafen

(55)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method:
Year: **GLP:**
Test substance:
Remark: Nach Applikation von unverduennter 2-Ethylhexansaeure (0.001 ml) wurden Nekrosen der Cornea festgestellt.
Source: BASF AG Ludwigshafen

(37)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: other: Smyth Carpenter
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen
(57)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen
(38) (58)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen
(40)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.: not irritating
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1985 **GLP:** yes
Test substance: other TS

Remark: Stamm: Neuseelaender
Source: BASF AG Ludwigshafen
Test substance: Substanzreinheit 99%

(64)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method:
Year: **GLP:**
Test substance:
Remark: Nach Applikation von unverduennter 2-Ethylhexansaeure wurden Nekrosen der Cornea festgestellt.
Source: BASF AG Ludwigshafen

(37)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: other: BASF-Test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(40)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: other: no details reported
Year: **GLP:** no data
Test substance: other TS
Remark: A 5% solution in dimethyl sulphoxide was irritating, while a1% solution was said to show only trace injury. No further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(61)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.: not irritating
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1985 **GLP:** yes
Test substance: other TS
Remark: Stamm: Neuseeländer
Source: Hoechst AG Frankfurt/Main
Test substance: Substanzreinheit 99 %

(65)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.: not irritating
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1985 **GLP:** yes
Test substance: other TS
Remark: Stamm: Neuseeländer
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test substance: Substanzreinheit 99 %

(65)

5.3 Sensitization

-

5.4 Repeated Dose Toxicity

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 15 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine
Doses: 0.75; 1.5; 3 % im Futter
Control Group: yes, concurrent no treatment
Method: OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 5 maennl. und 5 weibl. Tieren. Die durchschnittl. Dosis wurde fuer die weibl. Tiere mit 756; 1411 und 2658 mg/kg/Tag und fuer die maennl. Tiere mit 706; 1351 und 2276 mg/kg/Tag angegeben. Waehrend des Versuchs trat keine Mortalitaet auf. Bei den weibl. Tieren der beiden hohen Dosisgruppen wurde z.T. ein durch Urin gelb verfaerbtes adominales Fell beobachtet. Die Koerpergewichtsentwicklung der Tiere der hohen Dosisgruppe war signifikant reduziert, das Gewicht der weibl. Tiere lag zu Versuchsende 14 % und das der maennl. Tier 24 % unter dem der Kontrolltiere. Auch bei den maennl. Tieren der 1.5 % Dosisgruppe konnte noch eine reduzierte Koerpergewichtsentwicklung festgestellt werden. Dosisabhaengig konnte ein signifikant erhoehtes Lebergewicht bei den Tieren beider Geschlechter festgestellt werden. Bei den Tieren der beiden hohen Dosisgruppen wurden Hepatocyten-Hypertrophien und koagulierende Nekrosen der Hepatocyten beobachtet. Nierenlaesionen wurden nicht festgestellt.
Source: BASF AG Ludwigshafen

(66)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 90 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: z.T. 28 Tage
Doses: 0.1; 0.5; 1.5 % im Futter
Control Group: yes, concurrent no treatment
NOAEL: .5 %
Method: other: in Anlehnung an The 2-Ethylhexanoic Acid Final Test Rule (51 FR 40329, Section 795.260; 06.11.1986)
Year: 1986 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 10 maennl. und 10 weibl. Tieren. In der hoechsten Dosisgruppe wurde zusaetzlich eine Satellitengruppe mitgefuehrt, die nach der 90 taegigen Behandlung noch weitere 28 Tage nachbeobachtet wurde. Die durchschnittliche Substanzaufnahme

lag bei den maennl. Tieren bei 61; 303 und 917 mg/kg/Tag bei den weiblichen Tieren bei 71; 360 und 1068 mg/kg/Tag.
Es wurde keine behandlungsbedingte Mortalitaet, sowie keine signifikanten klinischen oder opthalmologischen Veraenderungen festgestellt.
Die Futteraufnahme in der hoechsten Dosisgruppe war reduziert, normalisierte sich aber waehrend der Nachbeobachtungszeit. Das Koerpergewicht der Tiere war in den beiden hohen Dosisgruppen reduziert.
Leichte haematologische Veraenderungen in Form von geringerem Haemoglobingehalt in den Blutkoerperchen und einem geringeren mittleren Erythrocytenvolumen wurden festgestellt. Das Lebergewicht der Tiere der 0.5 % und 1.5 % Dosisgruppe war erhoeht, histologische Veraenderungen waren Hepatocyten- Hypertrophien und reduzierte cytoplasmatische Vakuolisierung. Die Cholesterinwerte der maennl. Tiere waren erhoeht. Urinuntersuchungen zeigten, dass das Urinvolumen der weibl. Tiere der hohen Dosisgruppe verringert war, und die Urindichte erhoeht war. Die Osmolaritaet des Urins entsprach jedoch der Kontrolle, dies zeigte, dass die Nieren den Urin normal konzentrierten.

Source: BASF AG Ludwigshafen

(67) (68)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 15 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine
Doses: 0.75; 1.5; 3 % im Futter (750, 1500, 3000 mg/kg bw)
Control Group: yes, concurrent no treatment
Method: OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 5 maennl. und 5 weibl. Tieren. Die durchschnittl. Dosis wurde fuer die weibl. Tiere mit 756; 1411 und 2658 mg/kg/Tag und fuer die maennl. Tiere mit 706; 1351 und 2276 mg/kg/Tag angegeben.
Waehrend des Versuchs trat keine Mortalitaet auf. Bei den weibl. Tieren der beiden hohen Dosisgruppen wurde z.T. ein durch Urin gelb verfaerbtes adominales Fell beobachtet. Die Koerpergewichtsentwicklung der Tiere der hohen Dosisgruppe war signifikant reduziert, das Gewicht der weibl. Tiere lag zu Versuchsende 14 % und das der maennl. Tier 24 % unter dem der Kontrolltiere. Auch bei den maennl. Tieren der 1.5 % Dosisgruppe konnte noch eine reduzierte Koerpergewichtsentwicklung festgestellt werden.
Dosisabhaengig konnte ein signifikant erhoehtes Lebergewicht bei den Tieren beider Geschlechter festgestellt werden. Bei den Tieren der beiden hohen Dosisgruppen wurden Hepatocyten-Hypertrophien und koagulierende Nekrosen der Hepatocyten beobachtet. Nierenlaesionen wurden nicht festgestellt.

Source: BASF AG Ludwigshafen

(66) (69)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 90 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: z.T. 28 Tage
Doses: 0.1; 0.5; 1.5 % im Futter (100, 500, 1500 mg/kg bw)
Control Group: yes, concurrent no treatment
NOAEL: = .1 %
LOAEL: = .5 %
Method: other: in Anlehnung an The 2-Ethylhexanoic Acid Final Test Rule (51 FR40329, Section 795.260; 06.11.1986)
Year: 1986 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 10 maennl. und 10 weibl. Tieren. In der hoechsten Dosisgruppe wurde zusaetzlich eine Satellitengruppe mitgefuehrt, die nach der 90 taegigen Behandlung noch weitere 28 Tage nachbeobachtet wurde. Die durchschnittliche Substanzaufnahme lag bei den maennl. Tieren bei 61; 303 und 917 mg/kg/Tag bei den weiblichen Tieren bei 71; 360 und 1068 mg/kg/Tag.
Es wurde keine behandlungsbedingte Mortalitaet, sowie keine signifikanten klinischen oder opthalmologischen Veraenderungen festgestellt.
Die Futteraufnahme in der hoechsten Dosisgruppe war reduziert, normalisierte sich aber waehrend der Nachbeobachtungszeit. Das Koerpergewicht der Tiere war in den beiden hohen Dosisgruppen reduziert.
Leichte haematologische Veraenderungen in Form von geringerem Haemoglobingehalt in den Blutkoerperchen und einem geringeren mittleren Erythrocytenvolumen wurden festgestellt. Das Lebergewicht der Tiere der 0.5 % und 1.5 % Dosisgruppe war erhoeht, histologische Veraenderungen waren Hepatocyten- Hypertrophien und reduzierte cytoplasmatische Vakuolisierung. Die Cholesterinwerte der maennl. Tiere waren erhoeht. Urinuntersuchungen zeigten, dass das Urinvolumen der weibl. Tiere der hohen Dosisgruppe verringert war, und die Urindichte erhoeht war. Die Osmolaritaet des Urins entsprach jedoch der Kontrolle, dies zeigte, dass die Nieren den Urin normal konzentrierten.
Source: BASF AG Ludwigshafen

(67) (70) (68)

Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 3 weeks
Frequency of treatment: daily
Post. obs. period:
Doses: 1000 mg/kg bodyweight (given as 2 % in food)
Control Group: no data specified
Method: other: specific examination of the liver for peroxisome proliferation and enzyme activities.
Year: **GLP:** no data
Test substance: other TS
Result: The treatment led to decreased weight gain, highly increasedliver weights and highly increased peroxisome proliferation and activities of liver catalase and carnitine acetyltransferase. The treatment led also to decreased levels of cholesterol and triglycerides in blood.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(71)

Species: rat **Sex:** male
Strain: Wistar
Route of admin.: drinking water
Exposure period: 20 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine
Doses: 100; 1000; 5000; 10000 mg/l
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:**
Test substance:
Result: Die durchschnittliche Ethylhexansaeureaufnahme lag bei 0.3; 33; 130 und 200 mg/Tag. Kein Effekt auf das Koerpergewicht wurde bei den behandelten Tieren festgestellt.
Es wurde waehrend der Versuchsdauer die Ausscheidung von Ethylhexansaeure im Urin gemessen und nach Versuchsende die Wirkung auf mitochondriale Carnitin-Acetyltransferase Aktivitaet und die Citrullin-Synthese in der Leber bestimmt. Die Ausscheidung von Ethylhexansaeure stieg sowohl dosisabhaengig wie auch mit der Versuchsdauer.
Zu Versuchende war die mitochondriale Carnitin-Acetyltransferase- Aktivitaet dosisabhaengig signifikant erhoeht und die Citrullin- Synthese signifikant gehemmt.
Source: BASF AG Ludwigshafen

(72)

Species: rat **Sex:** male
Strain: Wistar
Route of admin.: drinking water
Exposure period: 20 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine
Doses: 100; 1000; 5000; 10000 mg/l (9, 91, 455, 909 mg/kg bw)
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:**
Test substance:
Result: Die durchschnittliche Ethylhexansaeureaufnahme lag bei 0.3; 33; 130 und 200 mg/Tag. Kein Effekt auf das Koerpergewicht wurde bei den behandelten Tieren festgestellt.
Es wurde waehrend der Versuchsdauer die Ausscheidung von Ethylhexansaeure im Urin gemessen und nach Versuchsende die Wirkung auf mitochondriale Carnitin-Acetyltransferase Aktivitaet und die Citrullin-Synthese in der Leber bestimmt. Die Ausscheidung von Ethylhexansaeure stieg sowohl dosisabhaengig wie auch mit der Versuchsdauer.
Zu Versuchende war die mitochondriale Carnitin-Acetyltransferase- Aktivitaet dosisabhaengig signifikant erhoeht und die Citrullin- Synthese signifikant gehemmt.
Source: BASF AG Ludwigshafen

(72)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 15 Tage
Frequency of treatment: 11 Applikationen in 15 Tagen
Post. obs. period: keine
Doses: 200; 800; 1600 mg/kg
Control Group: yes, concurrent no treatment
Method: OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 5 maennl. und 5 weibl. Tieren.
In der 1600 mg/kg Dosisgruppe starben je 4 maennl. und 4 weibl. Tiere waehrend den ersten beiden Versuchstagen (1 maennl. und 2 weibl. im moribunden Zustand eingeschlaefert), je ein maennl. und ein weibl. Tier ueberlebten bis zu Versuchsende. In den anderen Versuchsgruppen trat keine Mortalitaet auf. Die beiden ueberlebenden Tiere der hohen Dosisgruppe wiesen einen schlechten Allgemeinzustand auf (Schwaeche, Lethargie, Untertemperatur, Speichelfluss, mit Urin verschmiertes Fell, nasale Porphyrinausscheidung, Tremor). Auch die Tiere der 800 mg/kg Dosisgruppe wiesen diese Symptome, nur schwaecher, auf. Die Koerpergewichtsentwicklung der beiden Tiere der hohen und

der maennl. Tiere der 800 mg/kg Dosisgruppe war reduziert. Die absoluten Lebergewichte der Tiere der beiden hohen Dosisgruppen und die relativen Lebergewichte der maennl. Tiere der beiden hohen Dosisgruppen und aller behandelten weibl. Tiere waren erhoeht. Bei den histologischen Untersuchungen wurden bei den Tieren der hohen Dosisgruppe, die waehrend der Behandlung starben, Leberlaesionen in Form von cytoplasmatischer Vakuolisierung und Degeneration der Hepatocyten festgestellt. Hepatocyten-Hypertrophie wurde bei den ueberlebenden Tieren der hohen Dosisgruppe beobachtet. Keine behandlungsbedingten Veraenderungen wurden bei den Tieren der anderen Dosisgruppen festgestellt.

Source: BASF AG Ludwigshafen

(73)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 15 Tage
Frequency of treatment: 11 Applikationen in 15 Tagen
Post. obs. period: keine
Doses: 200; 800; 1600 mg/kg
Control Group: yes, concurrent no treatment
Method: OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 5 maennl. und 5 weibl. Tieren.
In der 1600 mg/kg Dosisgruppe starben je 4 maennl. und 4 weibl. Tiere waehrend den ersten beiden Versuchstagen (1 maennl. und 2 weibl, im moribunden Zustand eingeschlaefert), je ein maennl. und ein weibl. Tier ueberlebten bis zu Versuchsende. In den anderen Versuchsgruppen trat keine Mortalitaet auf. Die beiden ueberlebenden Tiere der hohen Dosisgruppe wiesen einen schlechten Allgemeinzustand auf (Schwaeche, Lethargie, Untertemperatur, Speichelfluss, mit Urin verschmiertes Fell, nasale Porphyrinausscheidung, Tremor). Auch die Tiere der 800 mg/kg Dosisgruppe wiesen diese Symptome, nur schwaecher, auf. Die Koerpergewichtsentwicklung der beiden Tiere der hohen und der maennl. Tiere der 800 mg/kg Dosisgruppe war reduziert. Die absoluten Lebergewichte der Tiere der beiden hohen Dosisgruppen und die relativen Lebergewichte der maennl. Tiere der beiden hohen Dosisgruppen und aller behandelten weibl. Tiere waren erhoeht. Bei den histologischen Untersuchungen wurden bei den Tieren der hohen Dosisgruppe, die waehrend der Behandlung starben, Leberlaesionen in Form von cytoplasmatischer Vakuolisierung und Degeneration der Hepatocyten festgestellt. Hepatocyten-Hypertrophie wurde bei den ueberlebenden Tieren der hohen Dosisgruppe beobachtet. Keine behandlungsbedingten Veraenderungen wurden bei den Tieren der anderen Dosisgruppen festgestellt.

Source: BASF AG Ludwigshafen

(74) (75)

Species: mouse **Sex:** male
Strain: other: C57BL/6
Route of admin.: oral feed
Exposure period: 4 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine Angabe
Doses: 30 mg/Tier/Tag
Control Group: yes
Method:
Year: **GLP:**
Test substance:
Result: Die Autoren untersuchten die Wirkung von 2-Ethylhexansaeure auf folgende hepatischen Parameter:
- Das rel. Lebergewicht (Leber-/Koerpergewicht) war signifikant erhoeht
- Keine Wirkung wurde auf den mikrosomalen und cytosolischen Proteingehalt festgestellt.
- Die Aktivitaet der hepatischen, cytosolischen Expoxid-Hydrolase war signifikant erhoeht.
- Der Gehalt von hepatischer, cytosolischer Expoxid-Hydrolase bezogen auf mg cytosolisches Protein war um den Faktor 1.5 erhoeht.
- Die Trans-Stilbenoxid Hydrolase-Aktivitaet war in der mitochondrialen Fraktion leicht verringert, in der cytosolischen Fraktion signifikant erhoeht.
- Kein signifikanter Effekt konnte auf den mikrosomalen Cytochrom P450 Gehalt oder auf die cytosolische Glutathion-Transferase-Aktivitaet festgestellt werden.

Die Autoren diskutierten die Induktion der Epoxid-Hydrolase als Sekundaereffekt der Peroxisomen-Proliferation.
Source: BASF AG Ludwigshafen

(76) (77)

Species: mouse **Sex:** male
Strain: other: C57BL/6
Route of admin.: oral feed
Exposure period: bis zu 14 Tagen
Frequency of treatment: kontinuierlich
Post. obs. period:
Doses: 0.25; 0.5; 1; 2; 4 % im Futter
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:**
Test substance:
Result: Die Autoren untersuchten die Wirkung auf die verschiedenen Leberenzymaktivitaeten.
Die cytosolische und mikrosomale Epoxid Hydrolase Aktivitaet waren erhoeht, die cytosolische Epoxid Hydrolase Aktivitaet war in der 1 % Dosisgruppe, die mikrosomale in der 2 % Dosisgruppe am staerksten, mit einem Maximum nach 3 Tagen, erhoeht. Auch die Carnitnin-Acetyltransferase-Aktivitaet, die als Mass fuer Peroxisomen-Proliferation genommen wurde, war erhoeht. Wurde

die Behandlung abgesetzt, so entsprachen 4 Tage nach Behandlungsende die Enzymaktivitaeten wieder dem Normalwert. Der somatische Leberindex war nach 4 Tagen Behandlung leicht erhoeht, der Proteingehalt in den mitochondrialen, mikrosomalen und cytosolischen Fraktionen war unveraendert. Ein behandlungsbedingter Anstieg der Cytochrom-Oxidase-Aktivitaet wurde gemessen. Keine Wirkung auf die, an Entgiftungsreaktionen beteiligten, Cytochrom P450 Enzyme und Glutathiontransferasen wurde festgestellt.

Source: BASF AG Ludwigshafen

(78)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 15 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine
Doses: 0.75; 1.5; 3 % im Futter
Control Group: yes, concurrent no treatment
Method: OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 5 maennl. und 5 weibl. Tieren.
Ein Tier der 0.75 % Dosisgruppe starb nach starkem Gewichtsverlust am 7. Versuchstag.
Die maennl. Tiere der hoechsten Dosisgruppe nahmen waehrend den ersten 4 Versuchstagen an Gewicht ab, bis zum 7. Versuchstag normalisierte sich das Gewicht wieder und blieb bis zum Ende des Versuchs konstant und lag dann 19 % unter dem durchschnittlichen Gewicht der Kontrolltiere. Bei den weibl. Tieren der 3 % Dosisgruppe blieb das Gewicht annaehernd konstant und lag zu Versuchsende 20 % unter dem der Kontrolltiere. In der 1.5 % Dosisgruppe konnte kein signifikanter Unterschied in der Koerpergewichtsentwicklung festgestellt werden, ebenso in der 0.75 % Dosisgruppe, hier waren die Tiere sogar etwas schwerer.
Das absolute und relative Lebergewicht der maennlichen Tiere der 3 % und 1.5 % Dosisgruppen und der weibl. Tiere aller Versuchsgruppen war signifikant erhoeht.
Bei histologischen Untersuchungen der Tiere wurden in der hohen Dosisgruppe bei 2/5 maennl. und 1/5 weibl. Tieren verkleinerte Thymusdruesen und bei 4/5 maennl. und 2/5 eine verkleinerte Milz beobachtet. Die Leber von 2/5 weibl. Tieren war narbig. Keine Nierenlaesionen wurden festgestellt. Dosisabhaengig wurden Hepatocyten-Hypertrophien und koagulierende Nekrosen der Hepatocyten festgestellt. In der hohen Dosisgruppen wurden bei Tieren von beiden Geschlechtern Atrophien der Thymusrinde und des Milzmarks beobachtet.

Source: BASF AG Ludwigshafen

(79)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 90 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: z.T. 28 Tage
Doses: 0.1; 0.5; 1.5 % im Futter
Control Group: yes, concurrent no treatment
NOAEL: .1 %
Method: other: in Anlehnung an the 2-Ethylhexanoic Acid Final Test Rule (51 FR 40329, Section 795.260; 06.11.1986)
Year: 1986 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 10 maennl. und 10 weibl. Tieren. In der hoechsten Dosisgruppe wurde zusaetzlich eine Satellitengruppe mitgefuehrt, die nach der 90 taegigen Behandlung noch weitere 28 Tage nachbeobachtet wurde. Die durchschnittliche Substanzaufnahme lag bei den maennl. Tieren bei 180; 885 und 2728 mg/kg/Tag bei den weiblichen Tieren bei 205; 1038 und 3139 mg/kg/Tag. Es wurden keine behandlungsbedingte Mortalitaet, keine signifikanten klinischen, opthalmologischen und haematologischen Veraenderungen festgestellt.
Die Futteraufnahme in der hoechsten Dosisgruppe war reduziert, normalisierte sich aber waehrend der Nachbeobachtungszeit. Das Koerpergewicht der Tiere war in den beiden hohen Dosisgruppen reduziert.
Das Lebergewicht der Tiere der 0.5 % und 1.5 % Dosisgruppe war erhoeht, histologische Veraenderungen waren Hepatocyten- Hypertrophien und reduzierte cytoplasmatische Vakuolisierung. Die Cholesterinwerte waren erhoeht, die Triglyceridwerte reduziert.
Bei ca. 40 % der Tiere der hohen Dosisgruppe wurden histologische Veraenderungen des renalen tubulaeren Epithels festgestellt. Keine funktionellen Stoerungen der Nieren wurden beobachtet. Der NOEL wurde mit 0.1 % 2-Ethylhexansaeure im Futter angegeben.
Source: BASF AG Ludwigshafen

(80) (68)

Species: mouse **Sex:** male
Strain: other: C57BL/6
Route of admin.: oral feed
Exposure period: 4 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine Angabe
Doses: 30 mg/Tier/Tag (ca. 1500 mg/kg bw)
Control Group: yes
Method:
Year: **GLP:**
Test substance:
Result: Die Autoren untersuchten die Wirkung von 2-Ethylhexansaeure auf folgende hepatischen Parameter:
- Das rel. Lebergewicht (Leber-/Koerpergewicht) war signifikant erhoeht
- Keine Wirkung wurde auf den mikrosomalen und cytosolischen Proteingehalt festgestellt.
- Die Aktivitaet der hepatischen, cytosolischen Expoxid-Hydrolase war signifikant erhoeht.
- Der Gehalt von hepatischer, cytosolischer Expoxid-Hydrolase bezogen auf mg cytosolisches Protein war um den Faktor 1.5 erhoeht.
- Die Trans-Stilbenoxid Hydrolase-Aktivitaet war in der mitochondrialen Fraktion leicht verringert, in der cytosolischen Fraktion signifikant erhoeht.
- Kein signifikanter Effekt konnte auf den mikrosomalen Cytochrom P450 Gehalt oder auf die cytosolische Glutathion-Transferase-Aktivitaet festgestellt werden.

Die Autoren diskutierten die Induktion der Epoxid-Hydrolase als Sekundaereffekt der Peroxisomen-Proliferation.
Source: BASF AG Ludwigshafen

(76) (77)

Species: mouse **Sex:** male
Strain: other: C57BL/6
Route of admin.: oral feed
Exposure period: bis zu 14 Tagen
Frequency of treatment: kontinuierlich
Post. obs. period:
Doses: 0.25; 0.5; 1; 2; 4 % im Futter (375, 750, 1500, 3000, 6000 mg/kg bw)
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:**
Test substance:
Result: Die Autoren untersuchten die Wirkung auf die verschiedenen Leberenzymaktivitaeten.
Die cytosolische und mikrosomale Epoxid Hydrolase Aktivitaet waren erhoeht, die cytosolische Epoxid Hydrolase Aktivitaet war in der 1 % Dosisgruppe, die mikrosomale in der 2 % Dosisgruppe am staerksten, mit einem Maximum nach 3 Tagen, erhoeht. Auch die Carnitnin-Acetyltransferase-Aktivitaet, die als Mass fuer

Peroxisomen-Proliferation genommen wurde, war erhoeht. Wurde die Behandlung abgesetzt, so entsprachen 4 Tage nach Behandlungsende die Enzymaktivitaeten wieder dem Normalwert. Der somatische Leberindex war nach 4 Tagen Behandlung leicht erhoeht, der Proteingehalt in den mitochondrialen, mikrosomalen und cytosolischen Fraktionen war unveraendert. Ein behandlungsbedingter Anstieg der Cytochrom-Oxidase-Aktivitaet wurde gemessen. Keine Wirkung auf die, an Entgiftungsreaktionen beteiligten, Cytochrom P450 Enzyme und Glutathiontransferasen wurde festgestellt.

Source: BASF AG Ludwigshafen

(78)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 15 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine
Doses: 0.75; 1.5; 3 % im Futter (1125, 2250, 4500 mg/kg bw)
Control Group: yes, concurrent no treatment
Method: OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 5 maennl. und 5 weibl. Tieren.
Ein Tier der 0.75 % Dosisgruppe starb nach starkem Gewichtsverlust am 7. Versuchstag.
Die maennl. Tiere der hoechsten Dosisgruppe nahmen waehrend den ersten 4 Versuchstagen an Gewicht ab, bis zum 7. Versuchstag normalisierte sich das Gewicht wieder und blieb bis zum Ende des Versuchs konstant und lag dann 19 % unter dem durchschnittlichen Gewicht der Kontrolltiere. Bei den weibl. Tieren der 3 % Dosisgruppe blieb das Gewicht annaehernd konstant und lag zu Versuchsende 20 % unter dem der Kontrolltiere. In der 1.5 % Dosisgruppe konnte kein signifikanter Unterschied in der Koerpergewichtsentwicklung festgestellt werden, ebenso in der 0.75 % Dosisgruppe, hier waren die Tiere sogar etwas schwerer.
Das absolute und relative Lebergewicht der maennlichen Tiere der 3 % und 1.5 % Dosisgruppen und der weibl. Tiere aller Versuchsgruppen war signifikant erhoeht.
Bei histologischen Untersuchungen der Tiere wurden in der hohen Dosisgruppe bei 2/5 maennl. und 1/5 weibl. Tieren verkleinerte Thymusdruesen und bei 4/5 maennl. und 2/5 eine verkleinerte Milz beobachtet. Die Leber von 2/5 weibl. Tieren war narbig. Keine Nierenlaesionen wurden festgestellt. Dosisabhaengig wurden Hepatocyten-Hypertrophien und koagulierende Nekrosen der Hepatocyten festgestellt. In der hohen Dosisgruppen wurden bei Tieren von beiden Geschlechtern Atrophien der Thymusrinde und des Milzmarks beobachtet.

Source: BASF AG Ludwigshafen

(79) (81) (82)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 90 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: z.T. 28 Tage
Doses: 0.1; 0.5; 1.5 % im Futter (150, 750, 2250 mg/kg bw)
Control Group: yes, concurrent no treatment
NOAEL: .1 %
Method: other: in Anlehnung an the 2-Ethylhexanoic Acid Final Test Rule (51 FR40329, Section 795.260; 06.11.1986)
Year: 1986 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 10 maennl. und 10 weibl. Tieren. In der hoechsten Dosisgruppe wurde zusaetzlich eine Satellitengruppe mitgefuehrt, die nach der 90 taegigen Behandlung noch weitere 28 Tage nachbeobachtet wurde. Die durchschnittliche Substanzaufnahme lag bei den maennl. Tieren bei 180; 885 und 2728 mg/kg/Tag bei den weiblichen Tieren bei 205; 1038 und 3139 mg/kg/Tag. Es wurden keine behandlungsbedingte Mortalitaet, keine signifikanten klinischen, opthalmologischen und haematologischen Veraenderungen festgestellt.
Die Futteraufnahme in der hoechsten Dosisgruppe war reduziert, normalisierte sich aber waehrend der Nachbeobachtungszeit. Das Koerpergewicht der Tiere war in den beiden hohen Dosisgruppen reduziert.
Das Lebergewicht der Tiere der 0.5 % und 1.5 % Dosisgruppe war erhoeht, histologische Veraenderungen waren Hepatocyten- Hypertrophien und reduzierte cytoplasmatische Vakuolisierung. Die Cholesterinwerte waren erhoeht, die Triglyceridwerte reduziert.
Bei ca. 40 % der Tiere der hohen Dosisgruppe wurden histologische Veraenderungen des renalen tubulaeren Epithels festgestellt. Keine funktionellen Stoerungen der Nieren wurden beobachtet. Der NOEL wurde mit 0.1 % 2-Ethylhexansaeure im Futter angegeben.
Source: BASF AG Ludwigshafen

(80) (70) (68)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 15 Tage
Frequency of treatment: 11 Applikationen in 15 Tagen
Post. obs. period: keine
Doses: 200; 800; 1600 mg/kg
Control Group: yes, concurrent no treatment
NOAEL: 800 mg/kg
Method: OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 5 maennl. und 5 weibl. Tieren. Ein maennl. Tier der 800 mg/kg Dosisgruppe und ein maennl. Tier der Kontrollgruppe starben waehrend der Versuchsdauer. Keine signifikante Wirkung auf die Koerper- gewichtsentwicklung der Tiere wurde festgestellt. In der hohen Dosisgruppe war das absolute und relative Lebergewicht der Tiere erhoeht. Bei pathologischen Untersuchungen wurden nur bei den maennl. Tieren der hohen Dosisgruppe Hepatocyten-Hypertrophien festgestellt. Keine weiteren Laesionen wurden beobachtet.
Source: BASF AG Ludwigshafen

(83)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 15 Tage
Frequency of treatment: 11 Applikationen in 15 Tagen
Post. obs. period: keine
Doses: 200; 800; 1600 mg/kg
Control Group: yes, concurrent no treatment
NOAEL: 800 mg/kg
Method: OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year: 1981 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 5 maennl. und 5 weibl. Tieren. Ein maennl. Tier der 800 mg/kg Dosisgruppe und ein maennl. Tier der Kontrollgruppe starben waehrend der Versuchsdauer. Keine signifikante Wirkung auf die Koerper- gewichtsentwicklung der Tiere wurde festgestellt. In der hohen Dosisgruppe war das absolute und relative Lebergewicht der Tiere erhoeht. Bei pathologischen Untersuchungen wurden nur bei den maennl. Tieren der hohen Dosisgruppe Hepatocyten-Hypertrophien festgestellt. Keine weiteren Laesionen wurden beobachtet.
Source: BASF AG Ludwigshafen

(83) (81)

Species: rabbit **Sex:** no data
Strain: no data
Route of admin.: oral unspecified
Exposure period: 5 Tage oder 12 Tage
Frequency of treatment: taeglich oder 10 Appl. waehrend 12 Tagen
Post. obs. period: keine
Doses: 1 ml einer 5 %igen waessrigen Loesung (Na-Salz)
Control Group: no
Method: other
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: Es wurden nur 2 Tiere in den Versuch eingesetzt. Ein Tier erhielt 5 das andere 10 Applikationen, beide Tiere starben. Bei dem Tier, das 5 Applikationen erhielt wurden Appetitlosigkeit nach der 3. und 5. Applikation Seitenlage und schliesslich Exitus festgestellt. Die Sektion war o.B.. Bei dem anderen Tier wurde bereits nach der 1. Applikation Seitenlage und Apathie beobachtet, nach der 10. Applikation starb das Tier. Bei der Sektion wurde eine leichtes Lungen-oedem festgestellt, sonst war die Sektion makroskop. o.B..
Source: BASF AG Ludwigshafen

(40)

Species: rabbit **Sex:** no data
Strain: no data
Route of admin.: oral unspecified
Exposure period: 2-4 Tage
Frequency of treatment: taeglich
Post. obs. period: keine
Doses: je 1 ml einer 10 % igen Loesung in Oel (Na-Salz)
Control Group: no
Method: other
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: Ein Tier starb bereits nach der 2. Gabe ohne zuvor Symptome zu zeigen. Die Lunge des Tieres war stark fluessigkeitshaltig, der Darm war stark durchblutet und der Magenfundus zeigte braune Pigmentierung.
Das 2. Tier starb nach 4 Applikationen, bereits nach der 2. Gabe wurden Benommenheit und Seitenlage beobachtet, weitere Symptome waren Durchfall, im Urin wurde vermehrt Eiweiss, im Sediment Erythro- und Leukocyten, sowie Harnstoffkristalle festgestellt. Die Sektion ergab im Magen und im Dickdarm Schleimhautblutungen.
Source: BASF AG Ludwigshafen

(40)

Species: rabbit **Sex:** no data
Strain: no data
Route of admin.: oral unspecified
Exposure period: 5 Tage oder 12 Tage
Frequency of treatment: taeglich oder 10 Appl. waehrend 12 Tagen
Post. obs. period: keine
Doses: 1 ml einer 5 %igen waessrigen Loesung (Na-Salz) (ca. 25 mg/kg bw)
Control Group: no
Method: other
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: Es wurden nur 2 Tiere in den Versuch eingesetzt. Ein Tier erhielt 5 das andere 10 Applikationen, beide Tiere starben. Bei dem Tier, das 5 Applikationen erhielt wurden Appetitlosigkeit nach der 3. und 5. Applikation Seitenlage und schliesslich Exitus festgestellt. Die Sektion war o.B.. Bei dem anderen Tier wurde bereits nach der 1. Applikation Seitenlage und Apathie beobachtet, nach der 10. Applikation starb das Tier. Bei der Sektion wurde eine leichtes Lungen-oedem festgestellt, sonst war die Sektion makroskop. o.B..
Source: BASF AG Ludwigshafen

(40)

Species: rabbit **Sex:** no data
Strain: no data
Route of admin.: oral unspecified
Exposure period: 2-4 Tage
Frequency of treatment: taeglich
Post. obs. period: keine
Doses: je 1 ml einer 10 % igen Loesung in Oel (Na-Salz) (ca. 50 mg/kg bw)
Control Group: no
Method: other
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: Ein Tier starb bereits nach der 2. Gabe ohne zuvor Symptome zu zeigen. Die Lunge des Tieres war stark fluessigkeitshaltig, der Darm war stark durchblutet und der Magenfundus zeigte braune Pigmentierung.
Das 2. Tier starb nach 4 Applikationen, bereits nach der 2. Gabe wurden Benommenheit und Seitenlage beobachtet, weitere Symptome waren Durchfall, im Urin wurde vermehrt Eiweiss, im Sediment Erythro- und Leukocyten, sowie Harnstoffkristalle festgestellt. Die Sektion ergab im Magen und im Dickdarm Schleimhautblutungen.
Source: BASF AG Ludwigshafen

(40)

Species: cat **Sex:** no data
Strain: no data
Route of admin.: gavage
Exposure period: 1; 2 oder 9 Tage
Frequency of treatment: taeglich oder 7 Appl. waehrend 9 Tagen
Post. obs. period: keine
Doses: je 1 ml einer 20 %igen oder 1 %igen Loesung in Oel (Na-Salz)
Control Group: no
Method: other
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: Die beiden Tiere, die die hohe Konzentration erhielten starben nach der ersten oder 2. Gabe. Bei beiden Tieren war die Sektion makroskopisch ohne Befund.
Das Tier, das die niedere Dosierung erhielt erbrach nach der 7. Sondierung Gallenfluessigkeit. Am darauf folgenden Tag wurde ein schlechter Allgemeinzustand, schwankender Gang, Seitenlage und Exitus bei dem Tier beobachtet. Bei der Sektion wurden eine eitrig fibrinoese Pleuritis ueber dem rechten Lungenmittellappen und eine geringgradige Bronchopneumonie festgestellt.
Source: BASF AG Ludwigshafen

(40)

Species: cat **Sex:** no data
Strain: no data
Route of admin.: gavage
Exposure period: bis zu 58 Tagen
Frequency of treatment: an ca. 5 Tagen/Woche
Post. obs. period: keine
Doses: je 1 ml einer 1; 5: 10 %igen waessrigen Loesung (Na-Salz)
Control Group: no
Method: other
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: 1 %ig:
Ein Tier erhielt 25 Applikationen in 35 Tagen, ein weiteres 40 Applikationen an 58 Tagen. Beide Tiere ueberlebten den Versuch. Z.T. wurde Erbrechen und Durchfall bei den Tieren beobachtet. Das Blutbild war o.B. auch bei der Sektion der Tiere zu Versuchende konnten keine Veraenderungen festgestellt werden.
5 %ig:
Ein Tier starb nach der 2. ein weiteres nach der 3. Applikation, Symptome waren Gleichgewichtsstoerungen und Seitenlage. Die Sektion der Tiere war ohne Befund. Das dritte Tier ueberlebte alle 10 durchgefuehrten Applikationen. Auch bei diesem Tier wurden nach der 1. Applikation Gleichgewichtsstoerungen beobachtet, nach der 5. Applikation wurde dieser Effekt nicht mehr festgestellt. Im Blut des Tieres war sowohl die Zahl der Erythrocyten, wie auch Leukocyten signifikant erhoeht. 10 %ig:
Ein Tier wurde nur eingesetzt, es ueberlebte alle 17

Applikationen die in 25 Tagen vorgenommen wurden. Im Blutbild des Tieres wurde ein Anstieg der Eosinophilen und Lymphocyten festgestellt, sowie ein Abfall der Neutrophilen. Die Sektion war o.B..

Source: BASF AG Ludwigshafen

(40)

Species: cat **Sex:** no data
Strain: no data
Route of admin.: gavage
Exposure period: 1; 2 oder 9 Tage
Frequency of treatment: taeglich oder 7 Appl. waehrend 9 Tagen
Post. obs. period: keine
Doses: je 1 ml einer 20 %igen oder 1 %igen Loesung in Oel (Na-Salz) (ca. 100 or 5 mg/kg bw)
Control Group: no
Method: other
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: Die beiden Tiere, die die hohe Konzentration erhielten starben nach der ersten oder 2. Gabe. Bei beiden Tieren war die Sektion makroskopisch ohne Befund.
Das Tier, das die niedere Dosierung erhielt erbrach nach der 7. Sondierung Gallenfluessigkeit. Am darauf folgenden Tag wurde ein schlechter Allgemeinzustand, schwankender Gang, Seitenlage und Exitus bei dem Tier beobachtet. Bei der Sektion wurden eine eitrig fibrinoese Pleuritis ueber dem rechten Lungenmittellappen und eine geringgradige Bronchopneumonie festgestellt.

Source: BASF AG Ludwigshafen

(40)

Species: cat **Sex:** no data
Strain: no data
Route of admin.: gavage
Exposure period: bis zu 58 Tagen
Frequency of treatment: an ca. 5 Tagen/Woche
Post. obs. period: keine
Doses: je 1 ml einer 1; 5: 10 %igen waessrigen Loesung (Na-Salz) (ca. 5, 25, 50 mg/kg bw)
Control Group: no
Method: other
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: 1 %ig:
Ein Tier erhielt 25 Applikationen in 35 Tagen, ein weiteres 40 Applikationen an 58 Tagen. Beide Tiere ueberlebten den Versuch. Z.T. wurde Erbrechen und Durchfall bei den Tieren beobachtet. Das Blutbild war o.B. auch bei der Sektion der Tiere zu Versuchende konnten keine Veraenderungen festgestellt werden.
5 %ig:
Ein Tier starb nach der 2. ein weiteres nach der 3.

Applikation, Symptome waren Gleichgewichtsstoerungen und Seitenlage. Die Sektion der Tiere war ohne Befund. Das dritte Tier ueberlebte alle 10 durchgefuehrten Applikationen. Auch bei diesem Tier wurden nach der 1. Applikation Gleichgewichtsstoerungen beobachtet, nach der 5. Applikation wurde dieser Effekt nicht mehr festgestellt. Im Blut des Tieres war sowohl die Zahl der Erythrocyten, wie auch Leukocyten signifikant erhoeht. 10 %ig:
Ein Tier wurde nur eingesetzt, es ueberlebte alle 17 Applikationen die in 25 Tagen vorgenommen wurden. Im Blutbild des Tieres wurde ein Anstieg der Eosinophilen und Lymphocyten festgestellt, sowie ein Abfall der Neutrophilen. Die Sektion war o.B..

Source: BASF AG Ludwigshafen

(40)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA100, TA1535, TA1537, TA1538
Concentration: 4 ug/plate - 2500 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: in Anlehnung an Ames B.N. et al.: Proc.Nat.Acad.Sci, USA 70, 2281-2285 (1973) und Ames B.N. et al.: Mut.Res. 31, 347-364 (1975)
Year: 1975 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(84)

Type: Ames test
System of testing: Salmonella typhimurium TA100, TA1535, TA1537, TA1538
Concentration: 4 ug/plate - 2500 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: in Anlehnung an Ames B.N. et al.: Proc.Nat.Acad.Sci, USA 70,2281-2285 (1973) und Ames B.N. et al.: Mut.Res. 31, 347-364 (1975)
Year: 1975 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(84)

Type: Ames test
System of testing: Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538
Concentration: 4 - 2500 µg/Platte
Metabolic activation: with and without
Result: negative
Method: other: keine Angaben
Year: 1982 **GLP:** no
Test substance: other TS
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test substance: Substanzreinheit 99,2 %

(85)

Type: Ames test
System of testing: Echerischia coli WP2uvrA
Concentration: 4 - 2500 µg/Platte
Metabolic activation: with and without
Result: negative
Method: other: keine Angaben
Year: 1982 **GLP:** no
Test substance: other TS
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test substance: Substanzreinheit 99,2 %

(85)

Type: Ames test
System of testing: S. typhimurium TA 97, TA 98, TA 100, TA 1535
Concentration: not indicated
Metabolic activation: with and without
Result: negative
Method: other: modified plate incorporation test with hamster S9-mix
Year: **GLP:** no
Test substance: other TS
Remark: Toxicity to bacteria was observed at 3.3 mg/plate. No further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(86)

Type: Ames test
System of testing: S. typhimurium TA 98 and TA 100
Concentration: not indicated
Metabolic activation: with and without
Result: negative
Method: other: standard plate incorporation test
Year: **GLP:** no
Test substance: other TS
Remark: Toxicity was observed at 2.9 mg/plate. No further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(87)

Type: Ames test
System of testing: Salmonella typhimurium
Concentration:
Metabolic activation: no data
Result: negative
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(88)

Type: Ames test
System of testing: Salmonella typhimurium TA98, TA100
Concentration:
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(89)

Type: Ames test
System of testing: Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537
Concentration:
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:**
Test substance:
Source: BASF AG Ludwigshafen

(90)

Type: Bacterial gene mutation assay
System of testing: Escherichia coli WP2uvrA
Concentration: 4 ug/plate - 2500 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: in Anlehnung an Green M.H.L. and Muriel W.J., Mut. Res. 38, 3-32, (1976)
Year: 1976 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(84)

Type: Bacterial gene mutation assay
System of testing: Escherichia coli WP2uvrA
Concentration: 4 ug/plate - 2500 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: in Anlehnung an Green M.H.L. and Muriel W.J., Mut. Res. 38, 3-32,(1976)
Year: 1976 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(84)

Type: Cytogenetic assay
System of testing: CHO-Zellen
Concentration:
Metabolic activation: no data
Result: positive
Method:
Year: **GLP:**
Test substance:
Remark: Angaben zu Dosierungen, Zytotoxizitaet und pH-Wert Aenderungen fehlen in der nur tabellarisch dargestellten Studie.
Source: BASF AG Ludwigshafen

(91)

Type: Sister chromatid exchange assay
System of testing: human lymphocytes
Concentration: up to 360.5 mg/l
Metabolic activation: without
Result: ambiguous
Method: other: 48 hours exposure and scoring of 25 - 30 metaphases from each of duplicate cultures
Year: **GLP:** no data
Test substance: other TS
Remark: Only a minimal increase in SCE-frequency was induced by the treatment (below 1.5 fold increase) but the result was

considered positive by the author.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(92)

Type: Sister chromatid exchange assay
System of testing: CHO-Zellen
Concentration:
Metabolic activation: no data
Result: positive
Method:
Year: **GLP:**
Test substance:
Remark: Angaben zu Dosierungen, Zytotoxizitaet und pH-Wert Aenderungen fehlen in der nur tabellarisch dargestellten Studie.
Source: BASF AG Ludwigshafen

(91)

Type: other: Lymphocyt-3H-Thymidin Test
System of testing: C57BL/6J Maus Milz-Lymphocyten
Concentration:
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:**
Test substance:
Remark: Milz-Lymphocyten wurden +/- S9 mit 2-Ethylhexansaeure inkubiert, (1 - 2.5 h), waehrend der letzten 30 min. der Inkubation wurde die DNA durch Zugabe von Tritium markiert. Der Tritiumeinbau in die DNA wurde bestimmt.
Source: BASF AG Ludwigshafen

(89)

5.6 Genetic Toxicity 'in Vivo'

-

5.7 Carcinogenicity

-

5.8 Toxicity to Reproduction

Type: Fertility
Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: drinking water
Exposure Period: m: 12 Wochen + 21 Tage Paarungsdauer w: 2 Wochen + 21 Tage Paarungsdauer
Frequency of treatment: kontinuierlich
Premating Exposure Period
male: 12 Wochen
female: 2 Wochen
Duration of test:
Doses: 100; 300; 600 mg/kg/Tag
Control Group: yes, concurrent no treatment
Method: other
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Result: Bei den Tieren wurde waehrend der Behandlung keine Wirkung auf das Koerpergewicht oder auf die Futter- und Trinkwasseraufnahme festgestellt. Keine sichtbaren klinischen Symptome wurden festgestellt. Bei den maennl. Tieren wurden dosisabhaengig erhoehte relative Nieren- und Lebergewichte, sowie verminderte Serum-Triglycerid-, Cholesterin und Bilirubin-Werte gemessen.
Die Anzahl der Traechtigkeiten bezogen auf die Zahl der Paarungen waren in der hoechsten Dosisgruppe um 28 % reduziert; auch in den beiden niederen Dosisgruppen wurde dieser Effekt festgestellt. Der Hormonstatus der Tiere wurde nicht untersucht. Das relative Gewicht der Nebenhoden war bei den Tieren der hoechsten Dosisgruppe um 12 % erhoeht. Die Spermienzahl in den Nebenhoden war dagegen um 14 % reduziert. Die Motilitaet der Spermatozoen war in der 100 mg/kg Dosisgruppe um 37 % in der 600 mg/kg Dosisgruppe um 22 % vermindert. Die Wurfgroesse war in der hoechsten Dosisgruppe um 16 % reduziert. Es wurde kein Vergleich zu historischen Kontrollen durchgefuehrt.
Kein Effekt auf das Koerpergewicht der Nachkommen wurde beobachtet. Die Zahl der Nachkommen mit Knickschwanz war dosisabhaengig erhoeht. Auch die Zahl der Nachkommen mit Beinanomalien war bei den behandelten Tieren erhoeht. Die Behandlung hatte keinen Effekt auf die Stillzeit und den Laktationsindex. Bei den Nachkommen der beiden hohen Dosisgruppen wurde vermehrt Lethargie, Haematome und abnormal duennes Haar beschrieben. Auch eine verzoegerte Entwicklung (Oeffnung der Augen, Durchbruch der Zaehne, Haarwachstum) der Nachkommen der behandelten Tiere wurde beschrieben. "Grip and cliff"- Vermeidungsreflex waren verzoegert bei den Nachkommen der behandelten Tiere, kein Effekt wurde auf andere Verhaltensparameter festgestellt. Die Autoren bezeichnen die Ergebnisse als vorlaeufig und wollen weitere Untersuchungen durchfuehren.
Source: BASF AG Ludwigshafen

(93) (94)

Type: Fertility
Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: drinking water
Exposure Period: m: 10 Wochen + 21 Tage maximale Paarungsdauer w: 2 Wochen + 21 Tage maximale Paarungsdauer, Gestation und Lactation
Frequency of treatment: kontinuierlich
Premating Exposure Period
male: 10 Wochen
female: 2 Wochen
Duration of test: 19 Wochen
Doses: 100; 300; 600 mg/kg/Tag
Control Group: yes, concurrent no treatment
NOAEL Parental: = 300 mg/kg bw
NOAEL F1 Offspr.: = 100 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS
Result: Die Behandlung fuehrte bei den erwachsenen Tieren zu keinen sichtbaren Anzeichen von Toxizitaet oder Mortalitaet. Weder Futterverbrauch noch Wasserkonsum differierten zwischen den Gruppen vor der Verpaarung noch waehrend der Paarungszeit. Bei den traechtigen Tieren war der Wasserverbrauch leicht reduziert in der hoechsten Dosis. Das Koerpergewicht der maennlichen Tiere war nicht reduziert, aber die weiblichen Tiere zeigten bei 600 mg/kg ab Tag 7 der Gestation ein reduziertes Koerpergewicht und die Koerpergewichtszunahme waehrend der Gestation war statistisch signifikant reduziert. Das relative Gewicht des rechten Nebenhodends war in der heochsten Dosis erheoeht. Die Anzahl der Traechtigkeiten bezogen auf die Zahl der Paarungen waren in der hoechsten Dosisgruppe um 28 % reduziert; auch in den beiden niederen Dosisgruppen wurde dieser Effekt festgestellt. Der Hormonstatus der Tiere wurde nicht untersucht. Die Spermienzahl in den Nebenhoden war um 14 % reduziert. Das Verhaeltnis der beweglichen Spermatozoen war in der 100 mg/kg Dosisgruppe um 37 % in der 600 mg/kg Dosisgruppe um 22 % vermindert. Die Behandlung fuehrte zu einem dosisabhaengigen Verzoegerung der Befruchtung. Alle nicht traechtigen Tiere gehoerten der hoechsten Dosis an. Die Wurfgroesse war in der hoechsten Dosisgruppe um 16 % reduziert. Es wurde kein Vergleich zu historischen Kontrollen durchgefuehrt. Die Zahl der totgeborenen Nachkommen war unbeeinflusst, aber postnatale Todesfaelle waren bei den mit Ethylhexansaeure behandelten Jungtieren haeufiger. Kein Effekt auf das Koerpergewicht der Nachkommen wurde bei der Geburt beobachtet, verringerte sich aber bei 600 mg/kg wahrend der Laktationsphase. Die Zahl der Nachkommen mit Knickschwanz war dosisabhaengig erhoeht. Auch die Zahl der Nachkommen mit Beinanomalien war bei den mit 300 und 600 mg/kg behandelten Tieren erhoeht. Die Behandlung hatte keinen Effekt auf die Stillzeit und den Laktationsindex. Bei den Nachkommen der beiden hohen Dosisgruppen wurde vermehrt Lethargie, Haematome und abnormal duennes Haar beschrieben. Auch eine verzoegerte Entwicklung (Oeffnung der Augen, Durchbruch der Zaehne,

Haarwachstum) der Nachkommen der behandelten Tiere wurde beschrieben. Die Entwicklung der "Grip and cliff"-Vermeidungsreflexe waren verzoegert bei den Nachkommen der behandelten Tiere (ab 100 bzw. 600 mg/kg), kein Effekt wurde auf andere Verhaltensparameter festgestellt. Die histologische Untersuchung der Geschlechtsorgane der erwachsenen Tiere waren ohne auffaelligen Befunde.

Source: BASF AG Ludwigshafen

Test substance: 2-ethylhexanoic acid, 99,5% purity; neutralized with NAOH

(93) (94)

5.9 Developmental Toxicity/Teratogenicity

Species: rat **Sex:** female

Strain: Wistar

Route of admin.: drinking water

Exposure period: 6.-19. Traechtigkeitstag

Frequency of treatment: kontinuierlich

Duration of test: bis zum 20. Tag der Traechtigkeit

Doses: 100; 300; 600 mg/kg

Control Group: yes

NOAEL Maternalt.: 300 mg/kg bw

Method: other

Year: **GLP:** no data

Test substance: as prescribed by 1.1 - 1.4

Result: 21 bzw. 20 Muttertiere wurden in die Dosis- bzw. Kontrollgruppen eingesetzt. Kein signifikanter Effekt auf die Muttertiere wurde beschrieben, nur bei den Muttertieren der hoechsten Dosisgruppe war das Koerpergewicht um ca. 10 % reduziert.
Bei den Nachkommen der beiden hohen Dosisgruppen war das Gewicht leicht reduziert. Dosisabhaengig wurde eine Zunahme der skelettalen Missbildungen festgestellt. Haeufigste skelettale Missbildung war Klumpfuss, desweiteren wurden abnormale Knorpel in den Knoecheln, Fehlen der Fibula, Polydactylie, Skoliose und Lordose und zusaetzliche Rippen beschrieben. Dosisabhaengig wurden skelettale Variationen festgestellt. Viszerale Missbildungen wurden nur vereinzelt beobachtet, jedoch ausschliesslich bei behandelten Tieren. Die Autoren beurteilen die Wirkung von 2-Ethylhexansaeure als teratogen, auch im nicht maternal toxischen Bereich.

Source: BASF AG Ludwigshafen

(95)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: drinking water
Exposure period: day 6-19 of gestation
Frequency of treatment: continuously
Duration of test: up to day 20 of gestation
Doses: 0, 100, 300 and 600 mg/kg b.w.
Control Group: yes, concurrent no treatment
NOAEL Maternalt.: = 300 mg/kg bw
NOAEL Teratogen.: = 100 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS
Method: The following parameters were examined: maternal body weight, number of corpora lutea, uterus weight, number of implantation sites, number and sex of live and dead fetuses, resorptions, fetal weights, placental weights, external anomalies, skeletal and visceral malformations and variations.
Remark: 20-21 pregnant females were used per dose. The fetuses were examined on gestational day 20 for external visceral and skeletal malformations and variations. The substance was marginally toxic to the dams at 600 mg/kg, but not at a lower dose, since the mean term body weight was reduced by 11%. This dose was slightly fetotoxic as indicated by a 5-8% decrease in the mean fetal body weight both in males an females. No treatment related effects were observed in the number of implantations or live fetuses. At a dose of 100 mg/kg and above 2-ethylhexanoic acid, caused skeletal malformations (clubfoot, absence of fibula, polydactyly), while the development of visceral tissue was less affected. The number of affected fetuses increased in a dose dependent way (4.9, 8.9, and 15.3% of treated offspring at 100, 300 and 600 mg/kg vs. 2,4% in the controls; statistically significant at 300 mg/kg or higher).
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, 99.5% pure; neutralized with NAOH

(96)

Species: rat **Sex:** female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: vermutlich 6.-15. Tag der Traechtigkeit
Frequency of treatment: vermutlich taeglich
Duration of test:
Doses: 100; 250; 500 mg/kg/Tag
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:**
Test substance:
Remark: Maternale Toxizitaet wurde in der hoechsten Dosisgruppe beschrieben. Sowohl in der 250 mg/kg und 500 mg/kg Dosisgruppe wurden foetale Variationen beobachtet, wie auch Anzeichen von foetaler Toxizitaet. Es konnten jedoch in keiner Dosisgruppe behandlungsbedingte Missbildungen festgestellt werden. (Die Autoren wiesen zusaetzlich darauf hin, dass die F344 Ratten im Vergleich zu anderen Rattenstaemmen, z.B. Wistar oder Sprague Dawley, gegenueber 2-Ethylhexansaeure und analogen Substanzen sehr empfindlich sind.)
Source: BASF AG Ludwigshafen

(97) (68)

Species: rat **Sex:** female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 6. - 15. Tag der Traechtigkeit
Frequency of treatment: taeglich
Duration of test:
Doses: 100; 250; 500 mg/kg/Tag
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Die Versuchs- und Kontrollgruppen bestanden aus je 25 Muttertieren. Maternale Letalitaet trat nicht auf. Nur in der hoechsten Dosisgruppe wurden klinische Veraenderungen (Hypoaktivitaet, Ataxie, laute Respiration, ocularer Ausfluss und perioculare Verkrustung) bei den Tieren festgestellt. Keine Wirkung auf das maternale Koerpergewicht wurde festgestellt. Sowohl das absolute wie auch das relative Lebergewicht der Tiere der hoechsten Dosisgruppe war erhoeht. Die Zahl der Corpora lutea, der gesamten, lebenden und nicht lebenden Implantate pro Wurf und das Geschlechterverhaeltnis waren von der Behandlung unbeeinflusst. Das Geburtsgewicht der Foeten der hoechsten Dosisgruppe war signifikant reduziert. Kein behandlungsbedingtes Ansteigen der Zahl der Foeten mit Missbildungen wurde festgestellt. In den beiden hohen Dosisgruppen war die Zahl der Variationen (500 mg/kg: skelettal + visceral; 250 mg/kg: skelettal) erhoeht, es handelte sich meistens um verminderte skelettale Ossifikationen. Dies deutete auf eine foetotoxische Wirkung der Behandlung hin. Der NOEL fuer die maternale Toxizitaet wurde mit 250 mg/kg,

der NOEL fuer die foetotoxische Wirkung mit 100 mg/kg angegeben.

Source: BASF AG Ludwigshafen

(98)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: gavage
Exposure period: am 12. Tag der Traechtigkeit
Frequency of treatment: einmalig
Duration of test:
Doses: 6.25; 12.5 mmol/kg
Control Group: yes
Method:
Year: **GLP:**
Test substance:
Result: Die Kontrollgruppe und niedere Dosisgruppe bestanden aus 7 Muttertieren, die hohe Dosisgruppe aus 10 Muttertieren. In der hohen Dosisgruppe waren 12.9 % der Implantate tot oder resorbiert, in der niederen Dosis waren es 5.9 %. Das Koerpergewicht der Foeten der niederen Dosisgruppe war reduziert. in der hohen Dosisgruppe wiesen 67.8 % der ueberlebenden Foeten Missbildungen auf, in der niederen Dosisgruppe 0.8 % Die Missbildungen der Nachkommen der Tiere der hohen Dosisgruppe waren zu 20.9 % Hydronephrosen, sowie 10.1 % Herzdefekte, zu 15.5 % Missbildungen des Schwanzes, zu 51.2 % der Extremitaeten und 10.9 % andere Missbildungen.
Source: BASF AG Ludwigshafen

(99)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: gavage
Exposure period: am 12. Tag der Traechtigkeit
Frequency of treatment: einmalig
Duration of test: no data
Doses: 6.25; 12.5 mmol/kg (900, 1800 mg/kg b.w.)
Control Group: yes
Method:
Year: **GLP:**
Test substance:
Result: Die Kontrollgruppe und niedere Dosisgruppe bestanden aus 7 Muttertieren, die hohe Dosisgruppe aus 10 Muttertieren. In der hohen Dosisgruppe waren 12.9 % der Implantate tot oder resorbiert, in der niederen Dosis waren es 5.9 %. Das Koerpergewicht der Foeten der niederen Dosisgruppe war reduziert. in der hohen Dosisgruppe wiesen 67.8 % der ueberlebenden Foeten Missbildungen auf, in der niederen Dosisgruppe 0.8 % Die Missbildungen der Nachkommen der Tiere der hohen Dosisgruppe waren zu 20.9 % Hydronephrosen, sowie 10.1 % Herzdefekte, zu 15.5 % Missbildungen des Schwanzes, zu 51.2 % der Extremitaeten und 10.9 % andere Missbildungen.
Source: BASF AG Ludwigshafen

(99)

Species: rat **Sex:** female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: day 12 of gestation
Frequency of treatment: single treatment
Duration of test: up to day 20 of gestation
Doses: 12.5 or 15.625 mM/kg bodyweight (1800 or 2250 mg/kg b.w.)
Control Group: yes, concurrent vehicle
Method: other: 7 - 10 dams/group and 97 - 115 live fetuses were examined
Year: **GLP:** no data
Test substance: other TS
Method: The following parameters were examined: maternal survival, number of implantation sites, number of live/dead fetuses, resorptions, fetal weights, skeletal and visceral malformations, substance concentration in maternal plasma and muscle and in fetal homogenate, yolk sac and extrocoelomic fluid.
Sprague-Dawley and Wistar rats were compared.
Result: The treatment did not lead to maternal death but to increased frequency of resorptions and fetal deaths, increased incidences of malformations up to 100 % of live fetuses and decreased fetal weights.
Primarily cardiovascular and appendicular skeletal malformations were induced. No difference in the effect on the two rat strains was seen.
Substance concentrations in embryonic tissue were about three times as high as in maternal tissue or plasma.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Aldrich, Milwaukee, no further data.

(100)

Species: rat **Sex:** female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: day 6 - 15 of gestation
Frequency of treatment: daily
Duration of test: up to post delivery day 6 or up to day 20 of gestation
Doses: 0, 900 or 1200 mg/kg bodyweight/day
Control Group: yes, concurrent vehicle
Method: other: according to Chernoff/Kavlock or segment II study
Year: **GLP:** no data
Test substance: other TS
Method: The following parameters were recorded: maternal body weightand clinical signs, pup weight, number of live pups, perinatal pup loss, number of implantation sites, gross external, skeletal and visceral malformations.
Result: The treatment lead to dose related decreased body weights, increased mortality and clinical signs in dams, to decreasedpup weights, decreased number of live pups and increased perinatal loss.
The incidence of skeletal malformations was highly increasedin treated groups in up to 98 % of pups (lumbar ribs).

Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid 99 % pure from Aldrich Chemical Corporation, no further data.

(101)

Species: rat **Sex:** female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: day 6 - 15 of gestation
Frequency of treatment: daily
Duration of test: up to day 21 of gestation
Doses: 0, 100, 250 or 500 mg/kg bodyweight/day
Control Group: yes, concurrent vehicle
NOAEL Maternalt.: = 250 mg/kg bw
NOAEL Teratogen.: = 500 mg/kg bw
Method: other: 21-24 dams/litters and 179-195 fetuses were examined
Year: **GLP:** no data
Test substance: other TS
Method: The following parameters were examined: maternal bodyweight,maternal liver weight, resorptions, live and dead fetuses, fetal weight, gross external, skeletal and visceral malformations and variations.
Result: The treatment did not influence maternal mortality or maternal body weight. Clinical symptoms such as hypoactivity, ataxia, irritating effects to the eyes were observed at the highest dose. The treatment led to increased absolute and relative maternal liver weight. The number of corpora lutea, the number of dead and alive pups per litter, and the sex ratio was unchanged. Fetal toxicity occured as reduced fetal weights and increased resorptions at the highest dose level. At 250 mg/kg or higher slight, fetal toxicity was seen as reduced skeletal ossification. No significant increase in malformations or variations was seen at any dose level. According to the authors the NOEL for maternal toxicity was 250 mg/kg and the NOEL for fetal toxicity 100 mg/kg.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid 99.4 % pure from Union Carbide Corporation, no further data.

(102) (103) (104) (105)

Species: rabbit **Sex:** female
Strain:
Route of admin.: gavage
Exposure period: 6.-18. Tag der Traechtigkeit
Frequency of treatment: taeglich
Duration of test:
Doses: 25; 125; 250 mg/kg/Tag
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:**
Test substance:
Result: In den beiden hohen Dosisgruppen wurde maternale Toxizitaet beobachtet, es konnten jedoch keine behandlungsbedingten foetalen Variationen oder Missbildungen festgestellt werden.
Source: BASF AG Ludwigshafen

(97) (68)

Species: rabbit **Sex:** female
Strain: New Zealand white
Route of admin.: gavage
Exposure period: 6.-18. Tag der Traechtigkeit
Frequency of treatment: taeglich
Duration of test:
Doses: 25; 125; 250 mg/kg
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: In die Versuchs- und Kontrollgruppen wurden je 15 traechtige Tiere eingesetzt.
In den beiden hohen Dosisgruppen starb je ein Muttertier, in der 125 mg/kg Gruppe hatte ein Tier einen Abort. In der hoechsten Dosisgruppe wurde maternale Toxizitaet in Form von zeitweise verminderter Koerpergewichtsentwicklung und nicht signifikanten klinischen Veraenderungen (Hypoaktivitaet, Ataxie, geraeuschvolle Respiration, Keuchen, Husten) festgestellt. Zu Versuchsende konnte weder eine Wirkung auf das Uterusgewicht noch auf das relative oder absolute Koerpergewicht festgestellt werden. Keine behandlungsbedingte Wirkung wurde auf die Zahl der Corpora lutea, die Zahl der Implantationen pro Wurf (lebend, nicht lebend, total), das Geschlechterverhaeltnis und das foetale Koerper- gewicht festgestellt. Kein signifikantes Ansteigen der Zahl der Foeten mit Missbildungen oder Variationen konnte festgestellt werden. In dieser Studie wurden keine behandlungsbedingten embryotoxischen, foetotoxischen oder teratogenen Wirkungen festgestellt. Der NOEL fuer die fruchtschaedigende Wirkung wurde von den Autoren mit 250 mg/kg angegeben, der NOEL fuer die maternale Toxizitaet mit 25 mg/kg.
Source: BASF AG Ludwigshafen

(106)

Species: rabbit **Sex:** female
Strain: New Zealand white
Route of admin.: gavage
Exposure period: day 6 - 18 of gestation
Frequency of treatment: daily
Duration of test: up to day 29 of gestation
Doses: 0, 25, 125 or 250 mg/kg bodyweight/day
Control Group: yes, concurrent vehicle
NOAEL Maternalt.: = 25 mg/kg bw
NOAEL Teratogen.: = 250 mg/kg bw
Method: other: 15 dams, 11-15 litters and 92-126 fetuses were examined
Year: **GLP:** no data
Test substance: other TS
Method: The following parameters were examined: maternal body weightand liver weight, maternal mortality, fetal weight, resorptions, number of live/dead fetuses, gross external, skeletal and visceral malformations and variations. 15 pregnant animals were used per group.
Result: In each of the two high dose groups, one animal died. At 125 mg/kg one animal had an abortion. In addition, slight maternal toxicity was seen at 250 mg/kg as reduced weight gain, food consumption and hypoactivity. There were no adverse effects on fetal viability, growth or morphology at any dose level. According to the authors, the NOEL for maternal toxicity was 25 mg/kg and the NOEl for developmental toxicity > 250 mg/kg.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid 99.4 % pure from Union Carbide Corporation, no further data.

(107) (108) (109) (106)

Species: mouse **Sex:** female
Strain: NMRI
Route of admin.: i.p.
Exposure period: day 7 - 8 of gestation
Frequency of treatment: twice daily
Duration of test: up to day 18 of gestation
Doses: 500 mg/kg bodyweight
Control Group: yes, concurrent vehicle
Method: other: 9 - 20 litters and 100 - 212 fetuses/group were examined
Year: **GLP:** no data
Test substance: other TS
Method: The (R) and (S) enantiomers were compared with the mixture, the following parameters were examined: embryolethality, fetal weight and incidence of exencephaly.
Result: The treatment with the (R)-enantiomer led to increased embryolethality of 11 % versus 6 % in controls and to highly increased incidence of exencephaly of 59 % of live fetuses. Fetal weight was not affected by the treatment. The (S)-enantiomer was not and the mixture was only slightly effective.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Aldrich, Germany, no further data.

(110)

Species: mouse **Sex:** female
Strain: other: SWV or C57BL/6NCrlBR
Route of admin.: i.p.
Exposure period: day 7 - 10 of gestation
Frequency of treatment: once or twice daily
Duration of test: up to day 17.5 or 18 of gestation
Doses: 403 - 1037 mg/kg bodyweight
Control Group: yes, concurrent no treatment
Method: other: 3 - 22 litters per group were examined
Year: **GLP:** no data
Test substance: other TS
Method: In a pretest single s.c. injections were used, in the main tests 3 - 4 i.p. injections were applied. The following parameters were examined: maternal deaths, implants, resorptions, fetal deaths, incidence of exencephaly, gross external, skeletal and visceral malformations.
Result: The treatment led to high incidences of exencephaly up to 50% of live fetuses and also high incidences of other malformations. The (R)-enantiomer was much more effective than the (S)-enantiomer but not always control data were included. Substance concentrations in embryonal tissue approximated concentrations in maternal plasma and tissue. Negative controls were only partly included in the examinations and the results are partly conflicting.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Aldrich Chemical Corporation, no further data.

(111)

Species: rat **Sex:** female
Strain: no data
Route of admin.: oral unspecified
Exposure period: 12. Tag der Traechtigkeit
Frequency of treatment: einmalig
Duration of test:
Doses: 6.25; 12.5 mmol/kg
Control Group: no data specified
Method:
Year: **GLP:**
Test substance:
Result: In der hohen Dosisgruppe waren 13.4 % der Implantationen resorbiert oder tot, 66.7 % der ueberlebenden Foeten wiesen Missbildungen auf. Es handelte sich zu 6 % um cardiovasculaere Defekte, zu 6.2 % um Hydronephrosen, zu 8.3 % um Missbildungen des Schwanzes und zu 74.3 % um Missbildungen der Gliedmassen. In tabell. Form liegen zusaetzlich die embryotoxischen Wirkungen einer oralen Dosis von 6.25 mmol/kg vor. 6.2 % der Implantate waren resorbiert oder die Foeten wurden tot geboren. 1 % der ueberlebenden Foeten wiesen Missbildungen auf, bei denen es sich ausschliesslich um Hydronephrosen handelte.
Source: BASF AG Ludwigshafen

(112) (113)

Species: rat **Sex:** female
Strain: no data
Route of admin.: oral unspecified
Exposure period: 12. Tag der Traechtigkeit
Frequency of treatment: einmalig
Duration of test:
Doses: 6.25; 12.5 mmol/kg (900, 1800 mg/kg b.w.)
Control Group: no data specified
Method:
Year: **GLP:**
Test substance:
Result: In der hohen Dosisgruppe waren 13.4 % der Implantationen resorbiert oder tot, 66.7 % der ueberlebenden Foeten wiesen Missbildungen auf. Es handelte sich zu 6 % um cardiovasculaere Defekte, zu 6.2 % um Hydronephrosen, zu 8.3 % um Missbildungen des Schwanzes und zu 74.3 % um Missbildungen der Gliedmassen. In tabell. Form liegen zusaetzlich die embryotoxischen Wirkungen einer oralen Dosis von 6.25 mmol/kg vor. 6.2 % der Implantate waren resorbiert oder die Foeten wurden tot geboren. 1 % der ueberlebenden Foeten wiesen Missbildungen auf, bei denen es sich ausschliesslich um Hydronephrosen handelte.
Source: BASF AG Ludwigshafen

(112) (113)

Species: rabbit **Sex:** female
Strain: no data
Route of admin.: unspecified
Exposure period: day 8 - 16 of gestation
Frequency of treatment: daily
Duration of test: not indicated
Doses: 0.025 or 0.125 mg/kg bodyweight
Control Group: no data specified
Method: other: no details specified
Year: **GLP:** no data
Test substance: other TS
Remark: The study is only as abstract available.
Result: Reduced activity, breathing difficulty, failure of muscle coordination and deaths occurred in pregnant rabbits given 0.125 mg/kg. No adverse effects were seen at 0.025 mg/kg. Noevidence of fetotoxicity or teratogenicity was seen at any dose level. No further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-etylhexanoic acid, no further data.

(114)

5.10 Other Relevant Information

Type: adsorption
Remark: 2-Ethylhexansaeure wurde leicht durch die aeussere Haut absorbiert und fuehrte innerhalb von kurzer Zeit zu toedlichen Vergiftungen bei Ratten.
Die Ratten wurden mit der geschorenen Bauchhaut in einer Spezialwanne fixiert, die 2 ml konz. 2-Ethylhexansaeure enthielt. 10 min. Exposition wirkten bei 4 von 6 Tieren letal, 30 min. und laengere Expositionen fuehrten bei allen eingesetzten Tieren zum Tod. Symptome waren Benommenheit und Seitenlage.
Source: BASF AG Ludwigshafen

(40)

Type: Biochemical or cellular interactions
Remark: Die Autoren untersuchten die Wirkung von 2-Ethylhexansaeure auf die Peroxisomenproliferation in vivo und in vitro.
Im in vivo Versuch applizierten sie maennl. und weibl. Ratten 14 Tage 13.5 mmol 2-Ethylhexansaeure / kg / Tag per Schlundsonde und bestimmten danach im Leberhomogenat die hepatische Peroxisomenproliferation. Sie stieg um den Faktor 8 im Leberhomogenat der behandelten Tiere.
Die in vitro Tests wurden mit Hepatocyten von maennl. Alderley Park Wistar-derived Ratten durchgefuehrt. Die Hepatocyten wurden als Monolayer mit der Substanz 24 Stunden inkubiert. Hier wurde ein 14-facher Anstieg der Peroxisomenproliferation festgestellt.
Source: BASF AG Ludwigshafen

(115)

Type: Biochemical or cellular interactions
Remark: When rat liver mitochondria were incubated in vitro with 2-ethylhexanoic acid the oxidation of various substrates (succinate, glutamate, malate, alpha-ketoglutarate) was significantly reduced. The enzyme responsible for this effect was not identified.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Janssen Chimica, Belgium, no further data.

(116)

Type: Biochemical or cellular interactions
Remark: The effects of 2-ethylhexanoic acid on various enzymes in mouse liver was investigated. Male C57BL/6 mice received thesubstance for 4 or 10 days in food at 1 % (2000 mg/kg bodyweight). The treatment increased significantly peroxisomal palmitoyl-CoA oxidation, peroxisomal lauroyl-CoAoxidation and microsomal and cytosolic catalase activity.
Treated animals had significantly increased absolute and relative liver weights, reduced body weights and increased protein content in liver homogenates.
The (+) enantiomer was much more effective in all parametersthan the (-) enantiomer.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Fluka AG, Switzerland, no further

data.

(117)

Type: Biochemical or cellular interactions
Remark: Rat and mouse liver cytosolic glutathione S-transferase activity was greatly inhibited by 2-ethylhexanoic acid at concentrations between 1 and 10 mM. The substance was considered by the author to be a weak to moderate inhibitor.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Aldrich Chemical Corporation, no further data.

(118)

Type: Biochemical or cellular interactions
Remark: 2-ethylhexanoic acid was applied by gavage to Wistar rats orB6C3F1 mice daily for 14 days at dose levels of 150 - 1900 mg/kg body weight. Liver weights and liver histology as wellas the activities of peroxisome associated enzymes were determined.
The treatment led to (partly significant) increased liver weights and dose related increased peroxisomal á-oxidation in both species.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, from Sigma Chemical Company, no further data.

(119)

Type: Biochemical or cellular interactions
Remark: The induction of peroxisome proliferation in isolated hepatocytes by DEHA and its metabolites was investigated as the palmitoyl-CoA-dependent reduction of NAD+.
2-ethylhexanoic acid was examined as a major metabolite of DEHA using mouse, rat, guinea pig and marmoset hepatocytes. Among all the 6 substances tested 2-ethylhexanoic acid was by far the most potent inducer of peroxisome proliferation.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Sigma, no further data.

(120)

Type: Biochemical or cellular interactions
Remark: In mice the oral administration of 0.16 g/kg/day and above for 14 days gave evidence of a dose related increase in peroxisome proliferation as measured by palmitoyl CoA oxidation. At approximately 0.8 g/kg/Iday and above in the diet for 14 days or more increased liver weight was noted. No further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(121)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanoic acid has a marked effect on lipid metabolismcausing inhibition of triglyceride biosynthesis in intestinal mucosa. This leads to changes in absorption of fatty acids and cholesterol. No further details are reported.
Source: BASF AG Ludwigshafen

Test substance: 2-ethylhexanoic acid, no further data.

(122)

Type: Metabolism
Remark: Maennliche Wistar-Ratten erhielten 9 Wochen 2-Ethylhexansaeure im Trinkwasser (600 mg/kg/Tag). Die Autoren untersuchten die Ausscheidung von 2-Ethylhexansaeure im Urin. Neben 2-Ethylhexansaeure konnten andere Metaboliten im Urin detektiert werden. Hauptmetabolit war 2-Ethyl-1,6 -hexandicarboxysaeure, weitere Metaboliten waren 2-Ethyl-6-hydroxy-hexansaeure, 5 weitere hydroxylierte Metabolite, 2 Lactone, ungesaettigte 5,6-Dehydro-2-Ethylhexansaeure und das Glucuronidkonjugat der 2-Ethylhexansaeure.
Source: BASF AG Ludwigshafen

(123)

Type: Metabolism
Remark: The effect of 2-ethylhexanoic acid on liver metabolism was examined in rats after oral application of 577 or 1010 mg/kg bodyweight daily for 3 days. The higher dose led to a significant hepatomegaly and induction of cytochrome P450 and peroxisomal PCCoA oxidase. The glucuronidation of nopol and the bilirubin conjugation was enhanced by the treatment. The glucuronidation of 2-ethylhexanoic acid by rat liver microsomes was determined in vitro. The microsomal UGT glucuronidated (R) and (S) 2-ethylhexanoic acid with a Km of2.09 and 2.35 mM and a Vmax of 7.35 and 7.72 nmol/min x mg protein. The glucuronidation was determined with liver microsomes of various species (rat, rabbit, guinea pig, dog,monkey and human).
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Aldrich, no further data.

(124)

Type: Metabolism
Remark: 2-ethylhexanoic acid was applied to rats daily for 3 days at 550 mg/kg bodyweight. Liver weight and enzyme activities in liver homogenate were determined.
The treatment led to increased liver weight and increased total and specific cytochrome P450 (4A1). The substance did not influence lauric acid w-hydroxylase activity but did induce palmitoyl-CoA oxidase activity.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid from Aldrich, no further data.

(125)

Type: Metabolism
Method: Excretion balance studies in rats were conducted with singlehigh (500 mg/kg) and low (50 mg/kg) oral doses and repeated low oral dosing for 14 days or by single dermal dosing with 1 g/kg or single i.v. dose of 1 mg/kg.
Result: Recovery of radioactivity after 96 hours for high dose and low dose oral application was (respectively): urine 56.72 % and 56.48 %, feces 15.27 % and 13.01 % and exhaled air 0.28 and 0.25 %.
Recovery after repeated application of 50 mg/kg was: urine

59.68 %, feces 14.15 % and exhaled air 0.26 % (within 96 hours after application).
Recovery after dermal application of 1 g/kg was within 96 hours: urine 3.32 %, feces 0.57 % and exhaled air 0.43 %.
Recovery after i.v. application of 1 g/kg was within 96 hours: urine 53.28 %, feces 3.84 % and exhaled air 0.44 %.

Source: BASF AG Ludwigshafen

Test substance: 2-ethylhexanoic acid from Eastman Chemical Corporation and radiolabelled 2-ethylhexanoic acid from Wizard Laboratories,no further data.

(126)

Type: Toxicokinetics

Remark: Die Verteilung von 2-Ethylhexansaeure nach i.p. Applikation von 2-14C-Ethylhexansaeure wurde bei maennl. Balb/C-Maeusen und maennl. Wistar-Ratten bestimmt.
Die Maeuse erhielten je 5 uCi (spez. Aktivitaet 6.7 mCi/mmol) 2-Ethylhexansaeure. Nach 30 min., 2 und 6 Stunden wurden Ganzkoerper-Autoradiographien durchgefuehrt. Bei den Tieren wurde die hoechste Aufnahme von radioaktiver 2-Ethylhexansaeure in der Leber, den Nieren und im Blut detektiert, nur geringe Mengen an Radioaktivitaet konnten im Gehirn detektiert werden. Geringe Radioaktivitaetsmengen wurden in der Nase und den Speicheldruesen gemessen.
Den Ratten wurden 2 uCi/Tier 2-14C-Ethylhexansaeure appliziert. Nach 2 Stunden wurde die hoechste Radioaktivitaet im Blut der Tiere festgestellt, hohe Konzentrationen an Radioaktivitaet wurden auch in Leber und Nieren der Tiere gemessen. Auch bei den Ratten wurden nur geringe Radioaktivitaetsmengen im Gehirn gemessen. Die Radioaktivitaet im Koerper der Tiere war nach 6 Stunden wesentlich geringer, und nach 24 Stunden war kaum noch Radioaktivitaet im Koerper der Tiere messbar.

Source: BASF AG Ludwigshafen

(127)

Type: Toxicokinetics

Remark: Pharmakologische Studien wurden mit 2-Ethylhexansaeure (2EHA) an F344 Ratten durchgefuehrt.
Wurde radioaktiv markiertes 2EHA den Ratten oral einmalig in den Dosen 100 oder 1000 mg/kg appliziert, so wurde die hoechste Konzentration im Blut nach 15-30 min. detektiert. Die Radioaktivitaet wurde zum groessten Teil ueber den Urin ausgeschieden; in der niederen Dosis wurden 79.3 % ueber den Urin und 12.4 % ueber die Faeces waehrend 96 Std. ausgeschieden, in der hohen Dosis waren es 82.2 % und 6.7 %. Radioaktiv markiertes 2EHA wurde in der Dosierung von 100 mg/kg an Ratten oral appliziert, die zuvor ueber 14 Tage taeglich nicht markiertes 2EHA in der gleichen Dosierung erhielten. Bei diesen Tieren lag die Ausscheidung der Radioaktivitaet ueber den Urin bei 60.3 % und 14.9 % wurden in den Faeces ausgeschieden. Wurde radioaktiv markiertes 2EHA dermal in den Dosierungen 100 und 1000 mg 24 Std. okklusiv dermal appliziert, so wurde in der niederen Dosierung die hoechste 2EHA-Blutkonzentration nach 5.7 Std. gemessen. Die Ausscheidung ueber den Urin lag bei der niederen Dosierung bei 41.7 % in der hohen Dosierung bei

46.7 %; in den Faeces wurden 7.5 % bzw. 7.1 % ausgeschieden. Wurde nach dermaler Applikation von 1000 mg/kg 2EHA die Substanz nach 5 min. gruendlich entfernt, so wurden in Urin und Faeces nur unwesentliche Mengen an Radioaktivitaet gemessen, 0.2 % innerhalb von 96 Std.. Nach i.v. Applikation von 1 mg/kg radioaktiv markiertem 2EHA nahm die Radioaktivitaet im Blut exponentiell ab. 66.6 % der Radioaktivitaet wurden im Urin und 3.6 % in den Faeces waehrend 96 Std. ausgeschieden.

Source: BASF AG Ludwigshafen

(128)

Type: Toxicokinetics

Remark: Pharmakologische Studien wurden mit 2-Ethylhexansaeure (2EHA) an F344 Ratten durchgefuehrt.
Wurde radioaktiv markiertes 2EHA den Ratten oral einmalig in den Dosen 100 oder 1000 mg/kg appliziert, so wurde die hoechste Konzentration im Blut nach 15-30 min. detektiert. Die Radioaktivitaet wurde zum groessten Teil ueber den Urin ausgeschieden; in der niederen Dosis wurden 79.3 % ueber den Urin und 12.4 % ueber die Faeces waehrend 96 Std. ausgeschieden, in der hohen Dosis waren es 82.2 % und 6.7 %. Radioaktiv markiertes 2EHA wurde in der Dosierung von 100 mg/kg an Ratten oral appliziert, die zuvor ueber 14 Tage taeglich nicht markiertes 2EHA in der gleichen Dosierung erhielten. Bei diesen Tieren lag die Ausscheidung der Radioaktivitaet ueber den Urin bei 60.3 % und 14.9 % wurden in den Faeces ausgeschieden. Wurde radioaktiv markiertes 2EHA dermal in den Dosierungen 100 und 1000 mg 24 Std. okklusiv dermal appliziert, so wurde in der niederen Dosierung die hoechste 2EHA-Blutkonzentration nach 5.7 Std. gemessen. Die Ausscheidung ueber den Urin lag bei der niederen Dosierung bei 41.7 % in der hohen Dosierung bei 46.7 %; in den Faeces wurden 7.5 % bzw. 7.1 % ausgeschieden. Wurde nach dermaler Applikation von 1000 mg/kg 2EHA die Substanz nach 5 min. gruendlich entfernt, so wurden in Urin und Faeces nur unwesentliche Mengen an Radioaktivitaet gemessen, 0.2 % innerhalb von 96 Std.. Nach i.v. Applikation von 1 mg/kg radioaktiv markiertem 2EHA nahm die Radioaktivitaet im Blut exponentiell ab. 66.6 % der Radioaktivitaet wurden im Urin und 3.6 % in den Faeces waehrend 96 Std. ausgeschieden.

Source: BASF AG Ludwigshafen

(128)

Type: Toxicokinetics

Result: 2-ethylhexanoic acid was applied to rats as a single oral dose per gavage at 100 or 1000 mg/kg bodyweight. Within 24 hours 72 - 75 % was excreted in urine and 7 - 12 % in feces.Only minor amounts were excreted unchanged in urine (2 - 7 %), the major part was excreted as glucuronidate.
After a single intraveneous injection of 1000 mg/kg bodyweight 64 % was excreted in urine and 2 % in feces within 24 hours.
A single dermal application of 100 or 1000 mg/kg bodyweight approximately 30 % was excreted in urine and 7 % in feces within 24 hours. Only 2 - 3 % was excreted in urine

unchanged, the rest was glucuronidated.
Source: BASF AG Ludwigshafen
Test substance: Radiolabelled 2-ethylhexanoic acid, no further data.
(129)

Type: other: Review
Remark: Literaturstudie ueber die hepatische Wirkung von lipidsenkenden Substanzen. 2-Ethylhexansaeure wurden folgende Wirkungen zugeschrieben:
- hepatische Peroxisomenproliferation
- Hepatomegalie
- lipidsenkend

Source: BASF AG Ludwigshafen
(130)

Type: other: Review
Remark: Zusammenfassende Darstellung
Source: BASF AG Ludwigshafen
(131) (132) (133)

Type: other: Review
Remark: Zusammenfassung der toxikologischen Studien von "Union Carbide" ueber 2-Ethylhexansaeure bis 1984
Source: BASF AG Ludwigshafen
(134) (42)

Type: other: Review
Remark: Zusammenfassende Darstellung
Source: BASF AG Ludwigshafen
(131) (132) (133)

Type: other: Review
Remark: Zusammenfassung der toxikologischen Studien von "Union Carbide" ueber 2-Ethylhexansaeure bis 1984
Source: BASF AG Ludwigshafen
(134) (42)

Type: other: bacteriostatic/fungistatic effects
Remark: Die bakteriostatische und fungistatische Wirkung von 2-Ethylhexansaeure wurde untersucht. Die bakteriostatische Wirkung wurde an den Testbakterien Typhus, Paratyphus A + B, Bac. Gaertner, Bac. Breslau, Pseudomonas, Pyocyaneus, Coli II, Coli Melsungen, Proteus, Aureus Hoe, A. Melsungen, A. Nixe, Strept. Arons. Kn., Strept. Arons. H.II gezeigt. Die fungistatische Wirkung konnte an Aspergillus niger nachgewiesen werden, jedoch nicht bei den hautpathogenen Pilzen Trichophyton granulosum und Mikrosporum gypseum.
Source: BASF AG Ludwigshafen
(135)

Type: other: effect on embryonic development in fish
Remark: 2-ethylhexanoic acid led to a concentration dependent retardation of embryonic development in zebra fish embryos. The concentrations used and further details are not reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(136)

Type: other: effects of chemical mixtures
Remark: The additive effects of aliphatic acids including 2-ethylhexanoic acid on frog embryos (reported by Dawson et al. 1991) are discused as relevant for ecotoxicological and toxicological purposes because of their occurrence in the environment.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(137)

Type: other: environmental effects
Remark: The effects of 2-ethylhexanoic acid alone or in combination with other aliphatic carboxylic acids on developmental malformations of frog embryos were examined.
2-ethylhexanoic acid at concentrations between 22 and 88 mg/l induced dose dependent increased incidences of malformations like microcephaly, gut coiling or general edema. The mixtures of carboxylic acids showed a concentration additive response.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid >= 98 % pure from Sigma Chemical Corporation or Aldrich Chemical Corporation, no further data.

(138)

Type: other: environmental effects
Remark: 2-ethylhexanoic acid affected adversely the development and metamorphosis of the larvae of the freshwater polyp Hydra atconcentrations between 0.1 and 1 mM. No details of possible mechanisms are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(139)

Type: other: environmental effects of chemical mixtures
Remark: The effect of 2-ethylhexanoic acid alone or in combination with other carboxylic acids on the types of malformations induced in frog embryos was investigated.
As found in previous investigations the effect of carboxylicacids on total malformation induction was concentration additive. For specific malformations no definite correlationwas found. 2-ethylhexanoic acid alone induced only microcephaly and abnormal gut coiling while other acids induced also eye defects and generalized edema.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid >= 98 % pure from Aldrich Chemical Corporation, no further data.

(140)

Type: other: general toxicity
Remark: In rabbits no changes in liver or body weights were observedwhen the substance was given in the diet at doses of appr. 0.5 g/kg bodyweight for 10 weeks. No further details are reported.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(141)

Type: other: risk assessment
Remark: The risk of developmental defects at the NOAEL was determined using a teratogenicity study published by Ritter et al. (1989). The author came to the conclusion that even at the NOAEL in the study cited a risk of 0.8 % for teratogenic effects exists. The conclusion is unclear.
Source: BASF AG Ludwigshafen
Test substance: 2-ethylhexanoic acid, no further data.

(142)

5.11 Experience with Human Exposure

Remark: Es liegen keine Untersuchungsberichte vor.
Source: BASF AG Ludwigshafen

Remark: Case report on chemical burn of the cornea after exposure to ethylhexanoic acid treated by denuding technic.
Source: BASF AG Ludwigshafen

(143)

Remark: Exposure to 2-ethylhexanoic acid (EHA) was determined by urinanalysisof the parent chemical and its metabolites in Finnish sawmill workers. The main route for entrance of EHA is by breathing, because urinary concentration correlated linearly with the concentration of EHA in the air. There was no correlation between skin contamination an durinary concentrations. Highest concentrations were found immediately after the work shift.
Source: BASF AG Ludwigshafen

(144)

Remark: In nine sawmill workers with exposure to 2-ethylhexanoic acid urinary excretion was investigated. The men with lower exposure excreted 30 nmol EHA/mmol creatinine, whereas men with higher exposure excreted 1.8 ómol EHA/mmol creatinine.
Source: BASF AG Ludwigshafen

(145)

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7.1 Risk Assessment

-

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I U C L I D

D a t a S e t

Existing Chemical	ID: 126-73-8
CAS No.	126-73-8
EINECS Name	tributyl phosphate
EC No.	204-800-2
TSCA Name	Phosphoric acid tributyl ester
Molecular Formula	C12H27O4P

Producer Related Part	
Company:	OECD
Creation date:	08-APR-2005

Substance Related Part	
Company:	OECD
Creation date:	08-APR-2005

Memo:	OECD HPV Chemicals Programme, SIDS Dossier, approved at SIAM 12 (27-29 June 2001)

Printing date:	29-JUL-2005
Revision date:	
Date of last Update:	29-JUL-2005

Number of Pages:	92

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 Applicant and Company Information
-

1.0.2 Location of Production Site, Importer or Formulator
-

1.0.3 Identity of Recipients
-

1.0.4 Details on Category/Template
-

1.1.0 Substance Identification
-

1.1.1 General Substance Information

Substance type: organic
Physical status: liquid
Purity: = 100 - % w/w

11-MAY-2005

1.1.2 Spectra
-

1.2 Synonyms and Tradenames

Phosphoric acid, tributyl ester

05-NOV-1997

TBP

05-NOV-1997

TRI-N-BUTYL PHOSPHATE

08-APR-2005

1.3 Impurities

Remark: no impurities above normal regulatory levels (1%, 0.1%)
08-APR-2005

1.4 Additives

Remark: no data currently available
08-APR-2005

1.5 Total Quantity

Quantity: 100 - 500 tonnes produced in 1998

08-APR-2005

1.6.1 Labelling

Labelling: as in Directive 67/548/EEC
Symbols: (Xn) harmful
Specific limits: no
R-Phrases: (22) Harmful if swallowed
S-Phrases: (2) Keep out of reach of children
(25) Avoid contact with eyes

08-APR-2005

1.6.2 Classification

Classified: as in Directive 67/548/EEC
Class of danger: harmful
R-Phrases: (22) Harmful if swallowed

08-APR-2005

1.6.3 Packaging
-

1.7 Use Pattern

Type: type
Category: Non dispersive use

08-APR-2005

Type: use
Category: Solvents

08-APR-2005

Type: use
Category: other: aircraft hydraulic fluid

18-JUL-2005

Type: use
Category: other: plasticizer for cellulose acetate, nitrocellulose and

08-APR-2005

1.7.1 Detailed Use Pattern
-

1.7.2 Methods of Manufacture
-

1.8 Regulatory Measures
-

1.8.1 Occupational Exposure Limit Values

Type of limit: TLV (US)
Limit value: 2.2 mg/m3

08-APR-2005

1.8.2 Acceptable Residues Levels
-

1.8.3 Water Pollution

Remark: not applicable
08-APR-2005

1.8.4 Major Accident Hazards

Legislation: other

Remark: mot applicable
08-APR-2005

1.8.5 Air Pollution

Classified by: other

Remark: not applicable
08-APR-2005

1.8.6 Listings e.g. Chemical Inventories
-

1.9.1 Degradation/Transformation Products
-

1.9.2 Components
-

1.10 Source of Exposure

Remark: no information available
08-APR-2005

1.11 Additional Remarks

Memo: Remark: no data

08-APR-2005

1.12 Last Literature Search
-

1.13 Reviews
-

2.1 Melting Point

Value: < -70 degree C

Method: OECD Guide-line 102 "Melting Point/Melting Range"
Year: 1987
GLP: no data
Test substance: other TS: Tributyl phosphate

Remark: The melting point of tributyl phosphate was reported by Bayer AG on their 1987 MSDS to be -70 C.
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
18-JUL-2005 (109)

2.2 Boiling Point

Value: 130 degree C at 5 hPa

Method: OECD Guide-line 103 "Boiling Point/boiling Range"
Year: 1987
GLP: no data
Test substance: other TS: Tributyl phosphate

Method: Boiling point determination
Remark: The boiling point of tributyl phosphate was reported by Bayer AG on their 1987 MSDS to be 130 C @ 5 hPa.
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
11-MAY-2005 (109)

2.3 Density

Type: density
Value: .97 g/cm³ at 20 degree C

24-AUG-1992 (109)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: .008 hPa at 20 degree C

08-APR-2005 (109)

Value: .00000347 hPa at 25 degree C

Year: 1990
GLP: yes
Test substance: other TS: Tributyl phosphate

Method: Guideline Followed: U.S. EPA Guideline 796.1950
Test Type: Vapor Pressure Determination
Remark: Guideline D-63-9 to comply with U.S. EPA TSCA Section 4 for tributyl phosphate
The vapor pressure of tributyl phosphate was determined at 25 degree C using the gas saturation technique. The average vapor
pressure at 25 degree C was determined by averaging the results of
three separate tests using high (about 10 ml/minute) and low (about 5 ml/minute) flow rates.
Result: The results of the analyses gave a mean vapor pressure for tributyl phosphate at 25 degree C of 0.00000346 hPa (2.6 E-6

mm Hg).
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
11-MAY-2005 (4)

Value: 1 hPa at 97 degree C

08-APR-2005 (10)

Value: 10 hPa at 144 degree C

08-APR-2005 (10)

2.5 Partition Coefficient

log Pow: 2.5

GLP: no data

Remark: experimentally determined
08-APR-2005 (120)

log Pow: 3.5

Method: other (calculated)
GLP: no data

Method: Leo, A.: CLOGP-3.54 MedChem Software 1989.
Daylight, Chemical Information Systems, Claremont, CA
91711, USA
08-APR-2005 (32)

log Pow: 4

Year: 1979
GLP: no

Method: Test Type: Octanol/Water Partition Coefficient, Shake Flask Method
USEPA Guideline 796.1550
Remark: experimentally determined
The octanol/water partition coefficient was measured for two concentrations of tributyl phosphate. The test material was placed in 100 ml of 1-octanol, which was then added to 500 ml of purified water which was shaken for 48 hours. The mixture was then held for one week in a separatory funnel, after which aliquots of the aqueous phase were removed and extracted twice with methylene chloride. The extracts were analyzed for tributyl phosphate using gas chromatography.
Result: The octanol/water partition coefficient for tributyl phosphate was determined to be Log Kow = 4
Conclusion: Octanol/Water Partition Coefficient: Log Kow = 4
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
11-MAY-2005 (108)

2.6.1 Solubility in different media

Solubility in: Water
Value: .4 g/l at 20 degree C

Method: OECD Guide-line 105
Year: 1987
GLP: no data
Test substance: other TS: Tributyl phosphate

Method: Test type: Water Solubility Determination
Conclusion: The water solubility was determined to be 0.4 g/l @ 20 C.
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
11-MAY-2005 (109)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: > 150 degree C

Method: other: DIN 51376
GLP: no data

08-APR-2005 (109)

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Dissociation Constant
-

2.13 Viscosity
-

2.14 Additional Remarks
-

3.1.1 Photodegradation

Type: other: degradation by UV-radiation

Year: 1985
GLP: no data
Test substance: other TS: Tributyl phosphate

Remark: The stability of tributyl phosphate was determined in the presence of ultraviolet light using low and high pressure mercury lamps. The exposure period was one hour.
Result: The photodegradation was 85% after 1 hour.
Conclusion: Under UV light, tributyl phosphate degrades about 85% in 1 hour.
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
18-JUL-2005 (69)

3.1.2 Stability in Water

Method: EPA OTS 796.3500
Year: 1990
GLP: yes

Method: Test Type: Hydrolysis as a function of pH
Remark: A 30 day hydrolysis study was conducted in buffered solutions at pH 3, 7, and 11 under dark conditions at 25 degree C. The test substance was radiolabeled with 14 degree C. The test solutions were prepared at a nominal concentration

of 10 ppm. Duplicate test samples were collected and analyzed after days 0, 1, 7, 14, 22, and 30 days.
The samples were analyzed for total radioactivity using liquid scintillation counting and for degradation of tributyl phosphate with thin layer chromatography (TLC). A 1 ml subsample from each of the 30 day samples was analyzed for microbial activity. The half life of the test substance was calculated at the 3 pH.

Result: The radioactivity in all of the samples was shown to be greater than 90% tributyl phosphate. Unknown products were detected at insignificant levels and appears constant at all time points and pH. No microbial contamination was observed in any of the samples. There was no evidence of significant hydrolytic degradation of tributyl phosphate at any of the 3 pH. The substance proved stable at all 3 pH and a decline curve could not be established for any of the buffered systems. The 14C mass balance ranged from 101.9% to 116.0% of the initial test solution with a mean of 108%. THC plate recoveries ranged from 67.5% to 96.4% with a mean recovery of 85.6%.

Test substance: Tributyl phosphate, Lot #9B125, with a purity of 99.7%, was obtained from FMC Corporation 14C-Tributyl phosphate, with a purity of 97.6%, was obtained from Wizard Laboratories.

Conclusion: Tributyl phosphate was hydrolytically stable at pH 3, 7, and

11.
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
18-JUL-2005 (124)

3.1.3 Stability in Soil

Type: laboratory
Radiolabel: yes
Soil temperature: 25 degree C

GLP: no data
Test substance: no data

Remark: The adsorption/desorption properties of 14C-tributyl phosphate (9B-125, PL89-289, radiopurity 98%) were studied in three different soil types (silt loam, clay loam, sandy loam) at 25 degrees C. The adsorption of TBP reached an equilibrium after 48 hours in all soils using a 0.01M Ca(NO3)2 solution: soil ratio of 5:1. Definitive mean measured test concentrations ranged from 0.516 to 0.101 (0.516, 0.387, 0.300, 0.205 and 0.101) ug/mL. The mean 14C-material balances for all definitive test concentrations with silt loam, clay loam and sandy loam were 95.8%, 101% and 97.7%, respectively. The Freudlich constants (Kd) for silt loam, clay loam and sandy loam were 5.84, 7.72, and 3.02, respectively. The adsorption constants as a function of carbon (Koc) were 1460, 1188 and 378 for silt loam, clay loam and sandy loam, respectively. The Koc values indicate that TBP has low mobility in silty loam and clay loam soil types with a medium mobility in sandy loam types.
08-APR-2005 (59)

3.2.1 Monitoring Data (Environment)

Medium: air

Remark: Japan (industrial area): 3.1 - 41.4 ng/m3
(non-industrial): < 10 ng/m3

08-APR-2005 (30)

Medium: surface water

Remark:

place	concentration (ng/l)	number of measurements proof	analized	Year
Rhein	max. 3800			1990
Ruhr	600			1990
Emscher	3900			1990
Lippe	800			1990
Wupper	600			1989
Sieg	100			1984

Zuericher See	54 - 82	2	2	1973
Norwegen (River Nitaiva)	100 - 900	3	7	1979
Japan (Dogo Plein, Ozu Basin area)	ND - 187	4	10	1974
Japan	20 - 710	16	100	1975
Japan	6 - 580	39	117	1977
Japan (Osaka)	20 - 4500	12	13	1976
Japan (Tokyo)	60 - 2100	12	12	1978
Japan (Kitakyushu City)	5 - 36	8	16	1980
Japan (Niigata City)	140	1	1	1982

08-APR-2005 (30)

Medium: sediment

Remark:

place	concentration ug/kg	number of measurement proof	analyzed	year
Japan	1.0 - 350	34	100	1975
Japan	1.9 - 240	48	117	1977
Japan (Tokyo)				
river	0.9 - 7.7	13	15	1978
sea	1.7 - 2.6	3	3	1978
Japan (Kitakyushu City)	NN**	0	6	1980

08-APR-2005 (30)

Medium: biota

Remark: Fish : 1.1 - 26 ug/kg
Crustacea : 10 - 20 ug/kg
Birds : 20 - 250 ug/kg

08-APR-2005 (30)

3.2.2 Field Studies

-

3.3.1 Transport between Environmental Compartments
-

3.3.2 Distribution

Method: Calculation according Mackay, Level I

Remark:

air	11 %
water	58 %
soil	16 %
sediment	15 %

12-MAY-2005 (30)

Media: other: air, water, soil, sediment
Method: Calculation according Mackay, Level III
Year: 2001

Method: Guideline Followed: No Guideline Available
GLP: No
The distribution of tributyl phosphate was estimated using the Mackay Level III Model. The input values used in the model are as follows:
Molecular Weight: 266.32
Water Solubility: 0.4 g/l at 20 degrees C
Vapor Pressure: 0.000347 Pa at 25 degrees C
Log Kow: 4
Melting Point: -70 degrees C

Result:

-	Percent distribution in			
Emissions	Air	Water	Soil	Sediment
Air only - 1000 kg/hour	0.67	<0.3	99	0
Water only - 1000 kg/hour	0	63	23	14
Soil only - 1000 kg/hour	0	0	100	0
Combined - 1000 kg/hour (air, water, and soil compartments)	0	1	99	0

Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
18-JUL-2005 (83)

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 100 mg/l
Degradation: 77 % after 28 day(s)

Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"
Year: 1985
GLP: no
Test substance: no data

Remark: related to O2-demand
08-APR-2005 (10)

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 3.68 mg/l
Degradation: 92 % after 28 day(s)

Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1985
GLP: no
Test substance: no data

Remark: related to BOD
08-APR-2005 (10)

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 20 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: 89 % after 28 day(s)

Method: OECD Guide-line 301 E "Ready biodegradability: Modified OECD Screening Test"
Year: 1985
GLP: no
Test substance: other TS: Tributyl phosphate

Method: Test Type: Ready Biodegradability: Modified OECD Screening Test
Remark: Domestic activated sludge from a sewage treatment plant was placed in glass vessels with 1.5 liters of operating volume. Tributyl phosphate was added to vessels in the amount of either 3 or 13 mg/l and stirred with magnetic stirrers for 24 hour cycles, for up to 21 weeks. To measure degradation, a sample was drawn from each vessel immediately after mixing the samples and again once a week. The tributyl phosphate was extracted with hexane and quantified using gas chromatography. The efficiency of the extraction and analytical methods was determined prior to the conduct of the experimental part of the study. To confirm that the biodegradation was more than a slight modification of the parent molecule, a CO2 evolution study was conducted. By measuring the amount of carbon dioxide produced and comparing that to the theoretical yield based on carbon content and weight of the ester, an indication of the total biodegradation of the molecule was obtained. The evolution study utilized 19.4 mg tributyl phosphate per liter of incubate.
Result: The activated sludge biodegraded tributyl phosphate, when added at the rate of 3 mg/l, 96% in 13 weeks. When added at 13

mg/l, the biodegradation was 56% 21% in 21 weeks. In the CO2 evolution study, the % of the theoretical carbon dioxide was 30.4% in 7 days and 90.8% in 28 days, confirming the molecule is completely biodegraded.

Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
11-MAY-2005 (108)

Type: aerobic
Inoculum: activated sludge, domestic, adapted
Concentration: .2 mg/l related to Test substance
Degradation: = 91 % after 28 day(s)

Method: other: Method similar to OECD 301B
GLP: no
Test substance: no data

Remark: Biodegradation variable; ranged from 3% of theoretical to 91% of theoretical amount of carbon dioxide evolved in 28 days
08-APR-2005 (97)

Type: aerobic
Inoculum: activated sludge
Concentration: 30 mg/l related to Test substance
Degradation: = 0 - 40 % after 14 day(s)

Method: other: see remarks
GLP: no data
Test substance: no data

Remark: "Biodegradation test of chemcial substance by organisms etc." stipulated in the Order Prescribing the Items of the Test Relating to the ew Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds" "302C, Inherent Biodegradability: Modified MITI Test II" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
sludge conc: 100 mg/l related to BOD
08-APR-2005 (16)

Type: aerobic
Inoculum: activated sludge, domestic, adapted
Concentration: 3 mg/l related to Test substance
Degradation: > 96 % after 24 hour(s)

Method: other: Method similar to OECD 302-A
GLP: no
Test substance: no data

Remark: Biodegradation at 13 mg/L was 56% as loss of parent material
08-APR-2005 (96)

Type: aerobic
Inoculum: activated sludge, domestic, adapted
Concentration: related to Test substance
Degradation: = 50 % after 5 day(s)
Result: other

GLP: no
Test substance: no data

Method: other: River Die-away; Test material spiked into river water and time to 50% degradation determined
08-APR-2005 (98)

Type: aerobic
Inoculum: activated sludge
Degradation: ca. 30 % after 2 day(s)

GLP: no data
Test substance: no data

Remark: no details
08-APR-2005 (69)

Type: aerobic
Inoculum: activated sludge
Degradation: ca. 100 % after 2 day(s)

GLP: no data
Test substance: no data

Remark: acclimatization.
no details.
08-APR-2005 (69)

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation

Species: Carassius auratus (Fish, fresh water)
BCF: 6 - 11

Method: OECD Guide-line 305 D "Bioaccumulation: Static Fish Test"
GLP: no data

Remark: Carassius auratus: 0.8-2.8 g
Concentration: 1.7-3.5 mg/l
08-APR-2005 (110)

Species: Cyprinus carpio (Fish, fresh water)
Concentration: 60 µg/l
BCF: 5.5 - 10

Method: other: see remarks
GLP: no data
Test substance: no data

Remark: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcen-tration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
08-APR-2005 (16)

Species: Cyprinus carpio (Fish, fresh water)
Concentration: 6 µg/l
BCF: 6.9 - 20

Method: other: see remarks
GLP: no data
Test substance: no data

Remark: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcen-tration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
08-APR-2005 (16)

Species: Oryzias latipes (Fish, fresh water)
BCF: 11 - 49

Method: OECD Guide-line 305 D "Bioaccumulation: Static Fish Test"
GLP: no data

Remark: Concentration: 0.06-4.0 mg/l
08-APR-2005 (111)

Species: Oryzias latipes (Fish, fresh water)
BCF: 30 - 35

Method: OECD Guide-line 305 D "Bioaccumulation: Static Fish Test"
GLP: no data
Test substance: no data

Remark: Oryzias latipes: 0.1-0.2 g
Concentration: 2-4 mg/l
08-APR-2005 (110)

Species: Oryzias latipes (Fish, fresh water)
BCF: 16 - 27

Method: OECD Guide-line 305 E "Bioaccumulation: Flow-through Fish Test"
GLP: no data

Remark: Concentration: 0.1-0.84 mg/l
08-APR-2005 (30)

3.8 Additional Remarks

Remark: Degradation by bacteria (Pseudomonas diminuta) isolated from river water and adapted for two months
> 50 % after 2 h
100 % after 43 h
(Concentration: 2 mg/l, temperature: 40 degree C)
08-APR-2005 (74)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC0: 4.3 -
LC50: 13 -
LC100: 19 -

Method: other: Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA, Ecological Research Series EPA-660/3-75-009, April 1975, U.S. EPA-TSCA, 40 CFR, Part 797 (1985)
GLP: no data
Test substance: no data

Test condition: Temperature: 12 degree C
08-APR-2005 (24)

Type: semistatic
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 10 day(s)
Unit: mg/l Analytical monitoring: no
* : 13.5 -

GLP: no data
Test substance: no data

Remark: * threshold concentration
Embryo-larval toxicity test
Nominal concentration; without feeding;
25 degree C
08-APR-2005 (38)

Type: semistatic
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 50 day(s)
Unit: mg/l Analytical monitoring: no
* : 8.3 -

GLP: no data
Test substance: no data

Remark: * threshold concentration
Embryo-larval toxicity test
Nominal concentration; without feeding;
8 degree C
08-APR-2005 (38)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 144 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 11.4 -

Method: other: ISO 1975
GLP: no data
Test substance: no data

Test condition: pH 7.3 - 8.5
Temperature: 25 degree C
08-APR-2005 (38)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 10 -
LC100: 14 -

Method: other: Letale Wirkung beim Zebrabaerbling, UBA-Verfahrensvorschlag, Mai 1984, Letale Wirkung beim Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h
Year: 1985
GLP: no
Test substance: no data

Remark: geom. mean: 11.8
Nominal concentration
08-APR-2005 (10)

Type: static
Species: Carassius auratus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 8.8 -

GLP: no data
Test substance: no data

Test condition: Temperature: 25 degree C
08-APR-2005 (110)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 5.8 -
LC50: 7.6 -
LC100: 8.7 -

Method: other: DEV, L 15 (1976)

GLP: no
Test substance: no data

08-APR-2005 (72)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
NOEC: = 4.9 -
LC50: = 11 -

Method: other: method similar to OECD 203
Year: 1990
GLP: yes

Method: Guideline Followed: U.S. EPA 40 CFR 797 Guideline 797.1400
Test Type: Acute 96-hour flow-through toxicity test of tributyl phosphate to the rainbow trout (Oncorhynchus mykiss)
Species/Strain/Supplier: Rainbow trout (Oncorhynchus mykiss), Mt. Lassen Trout Farm, Red Bluff, California
Statistical Methods: Stephan et al. LC50 program, U.S. EPA, 1985.

Remark: One hundred and forty fish were divided into groups of 10 fish per vessel. They had a mean weight of 0.91 grams and a mean standard length of 41 mm when measured at the end of the test. A proportional dilution system was used to introduce tributyl phosphate solutions into the flow-through system. The test substance was diluted with dimethylformamide (DMF) to achieve nominal concentrations of 1.3, 2.5, 5.0, 10, and 20 mg/l. The solvent control group received 0.1 ml/l of DMF. Two replicate vessels per
dose group were used (20 fish per dose). Temperature, dissolved oxygen and pH were measured at 0, 48, and 96 hours. The concentration of the test substance was measured in the vessels at 0, 48, and 96 hours. The test substance samples were analyzed using gas-liquid chromatography and a nitrogen phosphorus detector.

Result: 24 hour LC50 = 13 mg/l; 48 hour LC50 = 11 mg/l.
Water conditions determined during the conduct of this test were: hardness, 44-46 mg/l as $CaCO_3$, alkalinity, 58 mg/l as $CaCO_3$, pH 7.4-7.8, and total organic carbon, < 1 mg/l. The mean measured concentrations of tributyl phosphate were 1.2, 2.1, 4.3, 9.3, and 19 mg/l which yielded about 90% of the nominal target concentrations. Measurements of tributyl phosphate in the diluter stock solutions showed the chemical

to very stable for the duration of the test. The temperature was maintained at 13 C and the dissolved oxygen was 8.2 to 9.0 mg/l. The 24, 48, and 96 hour LC50 was determined to be 13 mg/l. Complete mortality was observed at the dose of 19 mg/l. There was no mortality in the lower dose groups. Sublethal behavioral effects were observed in the 9.3 mg/l dose group as loss of equilibrium, erratic swimming, labored respiration, quiescence, and surfacing. The no-observable-effect level (NOEL) was determined to be 4.3 mg/l.

Test substance: Tributyl phosphate, lot number 9B125, 99.7% pure, was provided by FMC Corporation.

Conclusion: The measured 96-hour LC50 concentration to rainbow trout is 13

mg/l.
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
18-JUL-2005 (6)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 11.5 - 13.5

GLP: no data
Test substance: no data

Remark: Nominal concentration
measured concentration: 5 - 9 mg/l,
no details about control;
only 4 fish for each concentration.
Test condition: 15 degree C
18-JUL-2005 (39)

Type: static
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 9.6 -

GLP: no data
Test substance: other TS: no data

Test condition: Temperature: 25 degree C
08-APR-2005 (110)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: = 3.2 -
LC50: = 6.4 -

Method: other: method similar to OECD 203
GLP: yes
Test substance: no data

Remark: 24 hour LC50=10 mg/l; 48 hour LC50=9.6 mg/l
08-APR-2005 (3)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)

Unit: mg/l Analytical monitoring:
LC50: 4.2 -

GLP: no data
Test substance: no data

Remark: Nominal concentration
Test condition: 20 degree C
08-APR-2005 (37)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 8.2 -

GLP: no data
Test substance: no data

Remark: Nominal concentration
Test condition: 15 degree C
08-APR-2005 (37)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 11.8 -

GLP: no data
Test substance: no data

Remark: Nominal concentration
Test condition: 10 degree C
08-APR-2005 (37)

Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 4.5 -

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
GLP: no data
Test substance: no data

08-APR-2005 (125)

Species: Oryzias latipes (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 4.5 -

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
GLP: no data
Test substance: no data

08-APR-2005 (125)

Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 14.2 -

Method: other: Japanese Industrial Standard (JIS K 0102-1986-71) "Testing methods for industrial waste water"
GLP: no data
Test substance: no data

08-APR-2005 (16)

Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 18 -

GLP: no data
Test substance: no data

08-APR-2005 (126)

Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 8.18 -
EC50 : 7.79 -

Test substance: as prescribed by 1.1 - 1.4

Remark: gas-liqid chromatography
Test condition: Temperature: 25.9 degree C
08-APR-2005 (62)

Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 11 -
EC50 : 6.56 -

GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Remark: gas-liqid chromatography
Test condition: Temperature: 26.7 degree C
08-APR-2005 (62)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 4.2 -

Method: OECD Guide-line 202
GLP: no data
Test substance: no data

08-APR-2005 (125)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no
EC0: 2.5 -
EC50: 5.8 -
EC100: 20 -

Method: other: Daphnien-Schwimmunfaehigkeits-Test, UBA-Verfahrensvorschlag Mai 1984, Bestimmung der Schwimmunfaehigkeit beim Wasserfloh Daphnia magna, EC0, EC50, EC100 24h, statisches System
Year: 1985
GLP: no
Test substance: no data

08-APR-2005 (10)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 12.8 -

Method: other: ISO (1975)
GLP: no data
Test substance: no data

08-APR-2005 (38)

Species: Daphnia magna (Crustacea)

Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 3.65 -

Method: other: ISO (1975)
GLP: no data
Test substance: no data

08-APR-2005 (38)

Species: Daphnia magna (Crustacea)
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 2.1 -

Method: other: ISO (1975)
GLP: no data
Test substance: no data

08-APR-2005 (38)

Species: Daphnia magna (Crustacea)
Exposure period: 14 day(s)
Unit: mg/l Analytical monitoring:
NOEC: 3.1 -

Method: OECD Guide-line 202
GLP: no data
Test substance: no data

08-APR-2005 (125)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: = 1.8 -
EC50: = 9 -

Method: other: method similar to OECD 202
GLP: yes
Test substance: no data

Remark: 24 hour EC50 = 23 mg/l
08-APR-2005 (5)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC0: 5 -
EC50: 30 -
EC100: 41 -

Method: other: static
GLP: no

Test substance: no data

08-APR-2005 (29)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC0: 7 -
EC50: 33 -
EC100: 58 -

Method: other: static
GLP: no
Test substance: no data

Remark: Nominal concentration
Test condition: Temperature: 20 - 22 degree C
08-APR-2005 (28)

Species: Daphnia magna (Crustacea)
Exposure period: 6 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 52 -

GLP: no data
Test substance: no data

08-APR-2005 (122)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC0: 9.3 -
EC50: 35 -

GLP: no data
Test substance: no data

Remark: Nominal concentration
08-APR-2005 (76)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 35 -

GLP: no data
Test substance: no data

08-APR-2005 (122)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: yes
NOEC: = .75 -
EC50: = 2.6 -

Method: other: U.S. EPA 40 CFR 797 Guideline 797.1300
Year: 1990
GLP: yes
Test substance: other TS: Tributyl phosphate, lot number 9B125, 99.7% pure, was provided by FMC Corporation.

Method: Test Type: Acute 48-hour flow-through toxicity test of tributyl phosphate to Daphnia magna
Species/Strain/Supplier: Daphnia magna obtained from an in -house daphnid culture maintained at ABC Laboratories since 1977.
Statistical Methods: Stephan et al.EC50 program, U.S. EPA, 1985.
Remark: The test system consisted of seven sets of four replicate one liter test chambers, each containing five daphnids.
The seven sets were identified as either the negative control, solvent control, or one of the five dose levels of

tributyl phosphate. The test substance was diluted with the solvent dimethylformamide (DMF) to achieve nominal test concentrations of 0.48, 0.96, 2.0, 4.0, and 8.0 mg/l. The concentration of tributyl phosphate was measured at 0, 24, and 48 hours. The load factor was about 1 daphnid per 200 ml water. Water quality measurements were made for the water used in the study. The solvent control group received 0.1 ml/l of DMF. Temperature, dissolved oxygen and pH were measured at 0, 24, and 48 hours. The test chambers were maintained at 20 C. The concentration of the test substance was measured at 0, 24, and 48 hours. The water samples containing the test substance were analyzed using gas-liquid chromatography and a nitrogen phosphorus detector.
Result: Water conditions determined during the conduct of this test were: hardness, 174-178 mg/l as $CaCO_3$, alkalinity, 200-202 mg/l as $CaCO_3$, pH 8.2-8.4, and total organic carbon, < 1 mg/l. The light cycle was 16 hours on, 8 hours off, with 30 minute transition periods. The mean measured concentrations of tributyl phosphate at 0, 24, and 48 hours were 0.32, 0.75, 1.8, 3.5, and 7.8 mg/l. These results yielded an average of 84, 12 % of the nominal target concentrations of 0.48, 0.96, 2.0, 4.0, and 8.0 mg/l. The 4, 24, and 48 hour EC50 values were >7.8, >7.8, and 2.6 mg/l, respectfully. The no observable effect concentration based on lack of immobility and other abnormal signs was 0.75 mg/l at 48 hours. One mortality was observed in the solvent control during this study. The dissolved oxygen concentration during the study was 8.7 to 8.9 mg/l, which were considered adequate and no supplemental aeration was necessary.
Measurements of tributyl phosphate in the diluter stock solutions showed the chemical to very stable for the duration of the test.
Conclusion: The measured 48-hour EC50 concentration to the daphnid is 2.6 mg/l (95% confidence limits of 2.2 and 3.1) and the no observable effect level is 0.75 mg/l.
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
11-MAY-2005 (5)

Species: Daphnia pulex (Crustacea)
Exposure period: 6 hour(s)

Unit: mg/l Analytical monitoring:
EC50: 93 -

GLP: no data
Test substance: no data

08-APR-2005 (122)

Species: Daphnia pulex (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 68 -

GLP: no data
Test substance: no data

08-APR-2005 (122)

Species: other: Gammarus pseudolimnaeus
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
NOEC: .52 -
LC50 : 1.7 -

Method: other: see remarks
GLP: no data
Test substance: no data

Remark: Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians, 795.120 of the Federal Register Guideline "Gammarid Acute Toxicity Test" and Standard Methods for Examination of Water and Wastewater (flow-through bioassay)
Length: 2 - 3 mm
Mortality and Immobilisation
Nominal concentration

08-APR-2005 (45)

Species: other: Hyalella azteca
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
NOEC: < 1.9 -
LC50 : 2.4 -

Method: other: see remarks
GLP: no data
Test substance: no data

Remark: Length: 1 - 2 mm
Nominal concentration
Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians, 795.120 of the Federal Register Guideline "Gammarid Acute Toxicity Test" and

Standard Methods for Examination of Water and Wastewater (flow-through bioassay).

08-APR-2005 (46)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Chlorella vulgaris (Algae)
Exposure period: 7 day(s)
Unit: mg/l Analytical monitoring:
EC50: 5 -

Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
GLP: no data
Test substance: no data

08-APR-2005 (125)

Species: Microcystis aeruginosa (Algae, blue, cyanobacteria)
Exposure period: 8 day(s)
Unit: mg/l Analytical monitoring: no
TT : 4.1 -

Method: other: cell multiplication inhibition test
GLP: no
Test substance: no data

Test condition: Temperature: 27 degree C
08-APR-2005 (26)

Species: Scenedesmus quadricauda (Algae)
Exposure period: 8 day(s)
Unit: mg/l Analytical monitoring: no
TT : 3.2 -

Method: other: cell multiplication inhibition test
GLP: no
Test substance: no data

Test condition: Temperature: 25 degree C
08-APR-2005 (26)

Species: Scenedesmus subspicatus (Algae)
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring:

Method: other: Scenedesmus-Zellvermehrungs-Hemmtest, DIN 38412 Teil 9, Bestimmung der Hemmwirkung von Wasserinhaltsstoffen auf Gruenalgen
GLP: no data
Test substance: no data

Remark: EC10 (biomass): 0.37; EC50 (biomass): 1.1
EC10 (growth rate): 0.92; EC50 (growth rate): 2.8

Species: Selenastrum capricornutum (Algae)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
NOEC: 2.2 -
EC50: 4.4 -

Method: other: static (ABC Protocol 8004-PMN)
GLP: no data
Test substance: no data

Test condition: Temperature: 24 degree C
08-APR-2005 (31)

Species: other algae: Chlorella emersonii
Exposure period: 2 day(s)
Unit: mg/l Analytical monitoring:
EC50: 5 - 10

GLP: no data
Test substance: no data

Test condition: Temperature: 25 degree C
08-APR-2005 (37)

Species: other aquatic plant: Phytoplankton (13 species)
Endpoint: growth rate
Exposure period: 14 day(s)
Unit: mg/l Analytical monitoring:
LOEC: 5 -
EC100 : 50 -

Method: other: Microtiter-Plates, visual evaluation
GLP: no data
Test substance: no data

Remark: LOEC 5 mg/l
08-APR-2005 (22)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 300 -

Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: 1985
GLP: no
Test substance: no data

Remark: direct weight
26-APR-2005 (10)

Type: aquatic
Species: activated sludge of a predominantly domestic sewage
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 100 -

Method: OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
GLP: no data

26-APR-2005 (126)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 16 hour(s)
Unit: mg/l Analytical monitoring: no
TT : > 100 -

GLP: no
Test substance: no data

Test condition: Temperature: 25 degree C
26-APR-2005 (27)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: Oncorhynchus mykiss (Fish, fresh water)
Endpoint: other: time to swim-up stage; survival, length and weight
Exposure period: 95 day(s)
Unit: mg/l Analytical monitoring: yes
NOEC: = .82 -
LOEC: = 1.7 -
MATC : = 1.2 -

Year: 1991
GLP: yes
Test substance: no data

Method: U.S. EPA. 1987. Fish Early Life Stage Toxicity Test (Amended. Federal Register, Vol. 52, No. 97/Wed., May 20, 1987; Part 797.1600 Amended: 19064-19066
Remark: Results based on measured concentrations.
18-JUL-2005 (2)

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Endpoint: other: EC50: based on immobilization; 21-Day LOEC: based on length, days to first brood and Y/D/D
Exposure period: 21 day(s)
Unit: mg/l Analytical monitoring: yes
NOEC: = .87 -
LOEC: = 2.1 -
EC50: > 2.1 -
MATC : = 1.35 -

Year: 1991
GLP: yes
Test substance: no data

18-JUL-2005 (1)

Species: Daphnia magna (Crustacea)
Exposure period: 21 day(s)
Unit: mg/l Analytical monitoring:
NOEC: 1.3 -

Method: other: "Verlaengerter Toxizitaetstest bei Daphnia magna (Bestimmung der NOEC fuer Reproduktionsrate, Mortalitaet und den Zeitpunkt des ersten Auftretens von Nachkommen; 21 d) Stand: 01.01.1984"
GLP: no data
Test substance: no data

Remark: Nominal concentration
measured value: 1.0 mg/l
26-APR-2005 (76)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Sediment Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants

GLP: no data
Test substance: no data

Remark: TBP is used as a constituent of cotton defoliants, producing leaf scorching, and is associated with an increase in the rate of leaf drying.
26-APR-2005 (68)

GLP: no data
Test substance: no data

Remark: TBP increases the drying rate of lucerne, resulting in excessive leaf loss.
26-APR-2005 (68)

GLP: no data
Test substance: no data

Remark: TBP applied by spraying as an emulsion (at a rate equivalent to 0.25 % of freshly harvested leaf/weight) doubled the drying rate f ryegrass leaves. Leaf respiration stopped and did not resume in the subsequent 4 days.
26-APR-2005 (68)

GLP: no data
Test substance: no data

Remark: TBP has been shown to damage the leaf surface and help herbicides penetrate bean leaves.
26-APR-2005 (68)

GLP: no data
Test substance: no data

Remark: There is no information on the effects of TBP on non-target plants, even at concentrations designed to produce desiccation of crop plants.
26-APR-2005 (68)

4.6.3 Toxicity to Soil Dwelling Organisms

Remark: No mortality was observed among two-spotted spider mites (Tetranychus urticae) fed TBP at a concentration of 2 g/kg.
18-JUL-2005 (68)

4.6.4 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks

Remark: TT 14 mg/l (Entosiphon sulcatum, 3 d)
TT 21 mg/l (Uronema Parduczi, 20 h)
TT 42 mg/l (Chilomonas parameaecium, 2 d)
26-APR-2005 (25)

Remark: EC50 20 mg/l (Tetrahymena pyriformis, 24 h)
26-APR-2005 (126)

5.0 Toxicokinetics, Metabolism and Distribution
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male
No. of Animals: 5
Vehicle: other: gavage
Doses: 464, 1000, 2150, and 4640 mg/kg
Value: = 1552 mg/kg bw

Method: other: Acute Oral Toxicity Test Guideline
Year: 1973
GLP: no
Test substance: other TS: Tributyl phosphate, lot number 3471, > 99% pure, was provided by Stauffer Chemical Co.

Method: Test Type: Acute Oral Toxicity Test in Rats
Analytical Monitoring: No
Exposure Period: Single Exposure
Statistical Methods: Not identified
Remark: = 1.6 ml/kg
Five male Sprague-Dawley rats, weighting from 210 to 230 grams, were assigned to each of four dose groups. Each animal received a single oral dose by gavage. The animals were observed daily for clinical signs of toxicity for 14 days after treatment. All animals underwent necropsy and gross examination.
Result: All 5 animals in the high dose group died by study day four. There was no mortality in any of the other 3 treatment groups. Clinical signs included slight to severe depression and excessive urination. No treatment-related gross lesions were found at necropsy. The acute oral LD50 in male rats was determined to be 3160 mg/kg with confidence limits of 2150-4639.
Conclusion: The acute oral LD50 in male rats is 3160 mg/kg (2150-4639).
Reliability: (2) valid with restrictions
Female animals not used. Documentation weak.

18-JUL-2005 (115)

Type: LD50
Species: rat
Value: 1600 - 3200 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (42)

Type: LD50
Species: rat

Value: = 3000 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (42) (114)

Type: LD50
Species: rat
Value: = 1400 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (70)

Type: LD50
Species: rat
Value: = 3350 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (73)

Type: LD50
Species: rat
Value: = 1390 mg/kg bw

GLP: no data
Test substance: no data

Remark: male rats
26-APR-2005 (93)

Type: LD50
Species: rat
Value: = 1530 mg/kg bw

GLP: no data

Remark: female rats
26-APR-2005 (93)

Type: LD50
Species: rat
Value: = 11265 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (47)

Type: LD50
Species: rat
Value: < 20000 mg/kg bw

GLP: no
Test substance: no data

26-APR-2005 (84)

Type: LD50
Species: mouse
Value: 400 - 800 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (42)

Type: LD50
Species: mouse
Value: = 1189 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (73)

Type: LD50
Species: mouse
Value: = 1240 mg/kg bw

Remark: male mice
26-APR-2005 (93)

Type: LD50
Species: mouse
Value: = 900 mg/kg bw

GLP: no data
Test substance: no data

Remark: female mice
26-APR-2005 (93)

Type: LD50
Species: hen
Value: = 1500 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (33)

Type: LD50
Species: hen
Value: = 1800 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (70)

Type: LD50

Species: hen
Value: = 1500 mg/kg bw

GLP: no data
Test substance: no data

26-APR-2005 (95)

5.1.2 Acute Inhalation Toxicity

Type: LC0
Species: rat
Exposure time: 6 hour(s)
Value: = 1.5 mg/l

GLP: no data

Remark: = 123 ppm
mortality: 0/3
strong skin and respiratory irritant
26-APR-2005 (48)

Type: LC50
Species: rat
Exposure time: 6 hour(s)
Value: > 42 mg/l

GLP: no data
Test substance: no data

Remark: with 3800 ppm (calculated): mortality 1/3, irritation = 42 mg/l 6h
with 350 ppm (calculated, = 4 mg/l): irritation, no mortalities (no further data).
26-APR-2005 (42)

Type: LC50
Species: rat
Exposure time: 1 hour(s)
Value: = 28 mg/l

GLP: no data
Test substance: no data

26-APR-2005 (50)

Type: LC50
Species: rat
Exposure time: 4 hour(s)
Value: > 4.242 mg/l

GLP: no data
Test substance: no data

Remark: maximum producable concentration = 4.242 mg/l, aerosol, analytical value.
2/5 male animals died, 0/5 female animals died
test according OECD guideline 403
26-APR-2005 (13)

Type: LC50
Species: rat
Exposure time: 1 hour(s)
Value: < 200 mg/l

GLP: no data
Test substance: no data

26-APR-2005 (58) (84)

Type: LC50
Species: mouse
Value: = 1.3 mg/l

GLP: no data
Test substance: no data

Remark: only calculated value, no experimental study
26-APR-2005 (73)

Type: other: LC
Species: cat
Exposure time: 5 hour(s)
Value: = 24.51 mg/l

GLP: no data
Test substance: no data

26-APR-2005 (44)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Value: > 3100 mg/kg bw

GLP: no data
Test substance: no data

18-JUL-2005 (70)

Type: LD50
Species: rabbit
Value: > 10000 mg/kg bw

GLP: no
Test substance: no data

10-MAY-2005 (84) (106)

Type: LD50
Species: guinea pig
Value: 9700 - 19400 mg/kg bw

GLP: no data
Test substance: no data

Remark: Application of 10-20 ml/kg bw
10-MAY-2005 (42)

Type: LD50
Species: rabbit
Value: > 10000 mg/kg bw

GLP: no
Test substance: no data

18-JUL-2005 (84) (106)

Type: LD50
Species: guinea pig
Value: 9700 - 19400 mg/kg bw

Remark: application of 10 - 20 ml/kg bw
Source: Bayer AG Leverkusen
31-JUL-1992 (42)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: rat
Route of admin.: i.p.
Value: 800 - 1600 mg/kg bw

GLP: no data
Test substance: no data

10-MAY-2005 (42)

Type: LD50
Species: rat
Route of admin.: i.p.
Value: = 251.2 mg/kg bw

GLP: no data
Test substance: no data

10-MAY-2005 (73)

Type: LD50
Species: mouse
Route of admin.: i.p.
Value: 100 - 200 mg/kg bw

GLP: no data
Test substance: no data

10-MAY-2005 (42)

Type: LD50
Species: mouse
Route of admin.: i.p.
Value: = 158.5 mg/kg bw

GLP: no data
Test substance: no data

10-MAY-2005 (73)

Type: other: LD
Species: rat
Route of admin.: i.p.
Value: = 1000 mg/kg bw

GLP: no data
Test substance: no data

Remark: 1000 or 5000 mg/kg bw were fatal within 1/2 to 4 hours. With 500 mg/kg bw coma for 24 hours, than recovery. with 50 or 100 mg neither behavioral nor pathological changes.

10-MAY-2005 (39)

Type: other: LD
Species: mouse
Route of admin.: s.c.
Value: = 3000 mg/kg bw

GLP: no data
Test substance: no data

10-MAY-2005 (44)

Type: other: LD
Species: rat
Route of admin.: i.v.
Value: 80 - 100 mg/kg bw

GLP: no data
Test substance: no data

Remark: 80 mg/kg sublethal, 100 mg/kg lethal, no cholinergic symptoms

10-MAY-2005 (121)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Result: slightly irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
GLP: no data
Test substance: no data

10-MAY-2005 (12)

Species: rabbit
Result: irritating

GLP: no data
Test substance: no data

Method: - concentrated tributyl phosphate: ear, occlusive 24 hours, soaked cotton swab or single painted ear: irritation
- 50 % in Lanoline: ear, occlusive, 24 hours: irritation
- 10 % in Lanoline: no irritation

10-MAY-2005 (66)

Species: rabbit
Result: highly irritating

Method: other: no data
GLP: no
Test substance: no data

10-MAY-2005 (56) (113)

Species: rabbit
Result: slightly irritating

Method: other: no data
GLP: no
Test substance: no data

10-MAY-2005 (57)

Species: rabbit
Result: highly irritating

GLP: no
Test substance: no data

Method: single dermal application of 500 mg/animal on intact or abraded skin of six rabbits.

10-MAY-2005 (53)

Species: rabbit
Result: irritating

GLP: no data
Test substance: no data

Method: The neat liquid or 10 % aqueous solutions applied on three to ten occasions to the intact or abraded skin: slight hyperaemia, tissue damage (no further data).
10-MAY-2005 (40)

Species: rabbit
Result: highly irritating

Method: other: exposure period 24 hours, no further data
GLP: no
Test substance: no data

10-MAY-2005 (84)

Species: guinea pig
Result: irritating

GLP: no data
Test substance: no data

Method: Skin, 24 hours contact under an impervious covering.
10-MAY-2005 (42)

Species: guinea pig
Result: highly irritating

GLP: no data
Test substance: no data

Method: covered contact with the neat liquid for 24 hours (no further data).
A 10 % solution in dimethyl phthalate was slightly irritating when applied to intact skin and moderately irritating when applied to abraded skin, whereas 2 % concentration caused no irritation (no further data).
10-MAY-2005 (41)

Species: human
Result: irritating

GLP: no data
Test substance: no data

Method: - concentrated tributyl phosphate:
arm, soaked cotton swab: irritation.
- 75 % in Lanoline:
arm, occlusive, 3 hours: irritation.
- 50 % in Lanoline:

arm, soaked cotton swab, 24 hours: mild irritation
- 10 % in Lanoline:
arm, soaked cotton swab, occlusive, 24 hours: no irritation

10-MAY-2005 (66)

Species: rat
Result: highly irritating

GLP: no data
Test substance: no data

Method: covered contact with the neat liquid for 5 days
10-MAY-2005 (107)

5.2.2 Eye Irritation

Species: rabbit
Result: slightly irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
GLP: no data
Test substance: no data

10-MAY-2005 (12)

Species: rabbit
Result: irritating

Method: other: no data
GLP: no
Test substance: no data

Remark: eye injury after 24 hour instillation
not irritant if washed out 4 seconds after instillation
10-MAY-2005 (51) (84) (113)

Species: rabbit
Result: slightly irritating

GLP: no
Test substance: no data

Method: instillation of 100 mg/animal, observation period min. 7 days
10-MAY-2005 (53)

Species: other: no data
Result: irritating

Method: other: no data
GLP: no data

Test substance: no data

Remark: transient irritation
10-MAY-2005 (42)

5.3 Sensitization

Type: Open epicutaneous test
Species: guinea pig
Result: not sensitizing

Method: other: test according EPA final test rule 1989, Test standard 798.4100
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: once weekly dermal application until a total of 3 applications, 14 day rest period, dermal challange on a virgin site.
10-MAY-2005 (54)

Type: Patch-Test
Species: human

GLP: no data
Test substance: no data

Remark: 53 volunteers, 15 applications of a formulation, said to contain less than 25 % tributyl phosphate, were made on alternate days. No volunteer gave local reactions 24 hours after the final patch, therefore no evidence of sensitization.
10-MAY-2005 (94)

Type: other: standard test
Species: guinea pig
Result: sensitizing

Method: other: standard sensitization test
GLP: no data
Test substance: no data

Remark: positive with 6 out of 15 animals (no further data).
10-MAY-2005 (42)

5.4 Repeated Dose Toxicity

Species: rat Sex: no data
Strain: no data
Route of administration: inhalation
Exposure period: 4 months
Frequency of treatment: 5 days/week, 5 hours/day
Post exposure period: 1 months
Doses: 5.1 or 13.6 mg/m3
Control Group: no data specified

GLP: no data
Test substance: no data

Remark: group size and purity not mentioned
Result: in the high concentration decrease of cholinesterase activity to 33 % after 3 months, effects on physiological and biochemical parameters esp. of the liver. The cholinesterase activity retained to normal in the postexposure period. In the low concentration no effect on cholinesterase activity (no further data).
10-MAY-2005 (73)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of administration: oral feed
Exposure period: 13 weeks
Frequency of treatment: daily (feeding study)
Post exposure period: no
Doses: 8, 40, 200, 1000 or 5000 mg/kg diet (0.6, 3, 15, 75 or 375 mg/kg bw/day)
Control Group: yes
NOAEL: 200 ppm

Method: other: U.S. EPA TSCA Subchronic Oral Toxicity Test Guideline
Year: 1985
GLP: yes
Test substance: other TS: Tributyl phosphate, lot number 2B-131, > 99% pure, was provided by FMC Corporation.

Method: Analytical Monitoring: Yes
Statistical Methods: Equality of means were evaluated using one-way analysis of variance (ANOVA) for body weight, food consumption, hematology, and clinical chemistry data; Bartlett's test was performed to determine group variances; Dunnett's test was used to determine significant differences.
Remark: 15 animals/sex/group
Species/Strain/Supplier: Sprague-Dawley Rats from Taconic Farms, Germantown, NY
This study was conducted to determine the effects of repeated exposure to tributyl phosphate on mortality, body weights, food consumption, hematology, clinical chemistry, and tissue morphology. Male and female rats were 30 days old at receipt, and were quarantined for one week prior to being placed in the study. Fifteen male and 15 female rats were

randomly allocated to each of six groups. Tributyl phosphate was administered daily by blending it into the diet. The control group received just rodent diet. Five male and female rats from each group were sacrificed after 45 days, at which time blood was collected for hematological evaluation and for measuring clinical
chemistry parameters. Tissues were taken for histopathology. The animals were maintained at 60-76 degree F with the humidity ranging between 35-72%. Water was available ad libitum. The actual concentration of the test substance in the diet was verified by analysis. All animals were observed daily for appearance and behavior, and for mortality. Body weights and food consumption were
determined weekly. Blood parameters were determined pre-test, at 45 days and at the end of the in-life phase (90 days). Hematology parameters measured include hematocrit, hemoglobin, erythrocyte count, leukocytes (total and differential), platelet count, mean corpuscular volume, and prothrombin time. Clinical chemistry parameters measured include ephosphatase, blood urea nitrogen, total bilirubin, SGPT, SGOT, SGGT, sodium, creatinine, phosphorus, potassium, albumin, total protein, and cholesterol. Brain, plasma, and erythrocyte cholinesterase activity was measured.
At the end of 90 days, all remaining animals were necropsied and examined for gross lesions. The following tissues were taken from each animal for examinaltion: brain, spinal cord (3 levels), pituitary, thyroid with parathyroids, thymus, trachea, lungs, heart, liver, spleen, pancreas, kidneys, adrenals, muscle, eyes, prostate, mammary gland,, skin, testes, ovaries, uterus, aorta, esophagus, stomach, duodenum, jejunum, ilium, colon, rectum, urinary bladder, and sciatic nerves. All tissues
were examined from the control and high dose animals. In addition, the livers and urinary bladders were examined from all other groups.

Result: No animals died during this study. Significant depression of body weight gain was seen only in the males and females in the high dose group (5000 ppm), occurring throughout the study, when compared to the body weights of control animals (25% and 30% depression for males and females, respectively). A significant decrease in food consumption was seen in the high dose animals during certain weeks, but not consistently. Measured dietary concentrations were 7.6,
39.2, 196, 980, and 4790 ppm, representing 95%, 98%, 98%, 98%, and 96% of the theoretical (nominal) concentrations. At the interim sacrifice, platelet counts were significantly increased in the 40 ppm males and 5000 ppm females. Mean corpuscular hemoglobin values were significantly decreased in the 1000 ppm females. None of
these findings were considered treatment-related. At termination, mean activated partial thromboplastin time was significantly elevated in the 5000 ppm males and this was considered treatment related.

Of the interim clinical chemistry measurements, the potassium value was lower in the 40 ppm males and plasma cholinesterase levels were higher in the 8 ppm females. Neither change was considered treatment related. Mean SGPT for the 5000 ppm males and SGGT values for the 1000 ppm and 5000 ppm males and 5000 ppm females were significantly elevated. This is considered treatment-related. At terminal sacrifice, SGOT values in the 8 ppm males and brain cholinesterase values in the 200 and 1000 ppm males was elevated, neither being treatment-related. Mean SGGT values for the 5000 ppm males and females, and mean albumin and calcium values for the 5000 ppm males were significantly elevated and these changes were considered treatment related. The only treatment-related histopathological finding was generalized transitional cell hyperplasia of the urinary bladders in the 1000 and 5000 ppm males and 5000 ppm females. There were no other treatment-related tissue changes in this study.
The no observable adverse effect level (NOAEL) was 200 ppm (13.8 mg/kg/day) for males and 1000 ppm (80.9 mg/kg/day) for females. The lowest observed adverse effect level (LOAEL) for tributyl phosphate in this study was 1000 ppm (68.2 mg/kg/day) for males and 5000 ppm (423.2 mg/kg/day) for females.

Conclusion: The NOAEL for males was 200 ppm (13.8 mg/kg/day) and for females was 1000 ppm (80.9 mg/kg/day).

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

18-JUL-2005 (34) (60)

Species: rat Sex: male
Strain: Wistar
Route of administration: oral feed
Exposure period: 3 months
Frequency of treatment: daily (feeding study)
Post exposure period: no
Doses: 500, 2000 or 10000 mg/kg diet (37.5, 150 or 750 mg/kg bw)
Control Group: yes

GLP: no data
Test substance: no data

Remark: purity and group size not mentioned
Result: dose-dependent depression of body weight gain, increments of liver, kidney and testis weight, and decrease in uterus weight, no changes in hematological analysis exept an increment on BUN value with high level of TBP (no further data).

10-MAY-2005 (93)

Species: rat Sex: male

Strain: Wistar
Route of administration: oral feed
Exposure period: 10 weeks
Frequency of treatment: daily (feeding study)
Post exposure period: no
Doses: 5000 or 10000 mg/kg diet (375 or 750 mg/kg bw)
Control Group: yes

GLP: no data
Test substance: other TS: purity > 97 %

Remark: 10-11 animals/group
Result: dose dependent decrease of body weight gain, decreased food consumption, decreased absolute weight of brain and kidneys, increase of total protein and cholesterol in the high dose group, increase of urea nitrogen and prolongation of blood coagulation in both treatment groups, decrease of activity of transaminases in both treatment groups, brain cholinesterase activity in the treatment groups was higher than in the control group, no change of cholinesterase activity in liver and serum.
10-MAY-2005 (102)

Species: rat Sex: male
Strain: Wistar
Route of administration: oral feed
Exposure period: 9 weeks
Frequency of treatment: daily (feeding study)
Post exposure period: no
Doses: 5000 mg/kg diet (375 mg/kg bw)
Control Group: yes

GLP: no data
Test substance: no data

Remark: 8 rats in the treatment group, 18 rats in the control group, purity not known
Result: decreased body weight gain, increased absolute and relative liver weight, unchanged hematologic values, increase of blood urea nitrogen, unchanged serum enzyme activity (transaminases, phosphatase, cholinesterase).
10-MAY-2005 (101)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of administration: gavage
Exposure period: 2 weeks
Frequency of treatment: daily

Post exposure period: no
Doses: 0.14 or 0.42 ml/kg bw (136 or 400 mg/kg bw)
Control Group: yes

GLP: no data
Test substance: other TS: purity 98.4 %

Remark: 10 animals/sex/group
Result: no overt signs of toxicity, decrease of Hb in high dose females, some changes of clinical chemistry parameters, increase of liver weight and liver to body ratio in high-dose groups, decrease of spleen weight in the high-dose female group, no gross morphological changes, one out of four male rats (high-dose group) showed microscopic degenerative changes in seminiferous tubules.

10-MAY-2005 (81)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of administration: gavage
Exposure period: 18 weeks
Frequency of treatment: 5 days/week
Post exposure period: no
Doses: 0.2 or 0.3-0.35 ml/kg bw (200 or 300-350 mg/kg bw)
Control Group: yes

GLP: no data
Test substance: other TS: purity 98.4 %

Remark: 12 animals/sex/group
Result: No overt signs of toxicity, decrease of body weight in high- dose male, no changes in hematological and biochemical parameters besides decrease of red blood cell acetylcholin- esterase, in high-dose female increase of liver weight and spleen weight, diffuse urothelial hyperplasia of urinary bladder in both sexes, no testicular changes.

18-JUL-2005 (79) (82)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of administration: gavage
Exposure period: 2 weeks
Frequency of treatment: daily
Post exposure period: no
Doses: 0.28 or 0.42 ml/kg bw (270 or 400 mg/kg bw)
Control Group: yes

GLP: no data
Test substance: other TS: purity 98.4 %

Remark: 10 animals/sex/group
Result: no overt signs of toxicity, reduction in conduction velocity of caudal nerve in high dose males, electron microscopic examination showed morphological changes such as retraction of Schwann cell processes surrounding unmyelinated fibres in high dose groups.
10-MAY-2005 (80)

Species: rat Sex: male
Strain: Wistar
Route of administration: gavage
Exposure period: 7 days
Frequency of treatment: daily
Post exposure period: no
Doses: 140 or 200 mg/kg bw
Control Group: no data specified

GLP: no data
Test substance: no data

Remark: purity and group size not mentioned
Result: marked increments of relative weights of liver and kidneys in accompany with increase of BUN value and tubular degeneration (no further data).
11-MAY-2005 (93)

Species: rat Sex: male
Strain: Wistar
Route of administration: gavage
Exposure period: one month
Frequency of treatment: daily
Post exposure period: no
Doses: 130 or 460 mg/kg bw
Control Group: no data specified

GLP: no data
Test substance: no data

Remark: purity and group size not mentioned
Result: marked depression of body weight gain and lethal cases by 20 and 40 % respectively, tubular damage (no further data).
11-MAY-2005 (93)

Species: rat Sex: no data
Strain: no data
Route of administration: dermal
Exposure period: chronic poisoning
Frequency of treatment: no data
Post exposure period: no data
Doses: no data
Control Group: no data specified

GLP: no data
Test substance: no data

Remark: NOEL: no data

purity and group size not mentioned
Result: effects on central nervous system, liver and kidneys (no further data).
11-MAY-2005 (73)

Species: mouse Sex: male/female
Strain: CD-1
Route of administration: oral feed
Exposure period: 4 weeks
Frequency of treatment: daily (feeding study)
Doses: 100, 1000, 5000 and 20000 mg/kg diet (15, 150, 750, 3000 mg/kg bw)
Control Group: yes

GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: 5/sex/group
Result: all animal receiving 20000 ppm in diet died or were sacrificed in a moribund condition (failure to eat, hypothermia, dyspnea, lethargy, tremor).
After 10 days the lowest dietary concentration was changed from 100 ppm to 10000 ppm. No mortality or clinical signs in the 1000, 5000, and 10000 ppm groups. Body weight changes in the 5000 and 10000 ppm groups, increases in liver weight and/or liver weight ratios in male mice at all dose levels and in female mice in the 5000 and 10000 ppm groups, decrease in absolute kidney weight in male mice (10000 ppm).
29-JUL-2005 (55)

Species: mouse Sex: male
Strain: other: ddy
Route of administration: oral feed
Exposure period: 3 months
Frequency of treatment: daily (feeding study)
Post exposure period: no
Doses: 500, 2000 and 10000 mg/kg diet (75, 300 and 1500 mg/kg bw)
Control Group: yes

GLP: no data
Test substance: no data

Remark: purity and group size not mentioned
Result: dose-dependent depression of body weight gain, increments of liver, kidney and testis weight, and decrease in uterus weight, no changes in hematological analysis exept an

increment on BUN value with high level of TBP (no further data).

11-MAY-2005 (93)

Species: mouse Sex: male/female
Strain: CD-1
Route of administration: oral feed
Exposure period: 3 month
Frequency of treatment: daily (feeding study)
Post exposure period: no
Doses: 500, 2000 and 8000 mg/kg diet (75, 300 and 1200 mg/kg bw/day)
Control Group: yes
NOAEL: 500 ppm

GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: 15/sex/group
Result: All animals survived, in the highest concentration body weight loss and reduced body weight gain with reduced food consumption and reduced fecal volume, elevation of absolute and relative liver weights with hepatocyte gypertrophy, slight to moderate epithelial hyperplasia of the urinary bladder, some slight hematological alterations and some effects on clinical chemistry parameters of liver function. In the middle concentration slight decrease of weight gains, elevated terminal ALT and AST in females and moderately elevated liver weights in both sexes, slight hepatocyte hypertrophy and minimal or slight epithelial hyperplasia of the urinary bladder.
NOEL: 500 ppm
120 mg/kg bw/day females
90 mg/kg bw/day males

18-JUL-2005 (21)

Species: rabbit Sex: no data
Strain: no data
Route of administration: inhalation
Exposure period: 4 months
Frequency of treatment: 5 days/week, 5 hours/day
Post exposure period: 1 month
Doses: 4.8 or 13.6 mg/m3
Control Group: no data specified

GLP: no data
Test substance: no data

Remark: group size and purity not mentioned
Result: in the high concentration decrease of cholinesterase activity to 33 % after 3 months, effects on physiological and biochemical parameters esp. of the liver. The cholinesterase activity retained to normal in the postexposure period. In the low concentration no effect on cholinesterase activity (no further data).

11-MAY-2005 (73)

Species: rabbit Sex: no data
Strain: no data
Route of administration: gavage
Exposure period: 14 days
Frequency of treatment: 7 applications
Post exposure period: no data
Doses: 100, 500 or 1000 mg/kg bw
Control Group: no data specified

GLP: no
Test substance: no data

Remark: purity and size of groups not mentioned
Result: with 1000 mg/kg transient excretion of protein with urine, no other effects
11-MAY-2005 (66)

Species: other: see remarks Sex: no data
Strain: no data
Route of administration: gavage
Exposure period: no data
Frequency of treatment: daily
Post exposure period: no data
Doses: 0.2 to 5 mg/kg/day
Control Group: no data specified

GLP: no data
Test substance: no data

Remark: NOEL: no data
rabbit and rat
purity and group size not mentioned
Result: liver necrosis, increased liver weight, in one of two studies increased kidney weight and tubulus dystrophia (no further data).
11-MAY-2005 (103) (127)

Species: other: see remarks Sex: no data
Strain: no data
Route of administration: dermal
Exposure period: no data
Frequency of treatment: no data

Post exposure period: no data
Doses: no data
Control Group: no data specified

GLP: no data
Test substance: no data

Remark: rat, guinea pig and rabbit
Result: purulent-necrotic fissures (no further data).
11-MAY-2005 (73)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA102 and TA2638 and Escherichia coli WP2/pKM101 and WP2 uvr/pKM101
Metabolic activation: with and without
Result: negative

Method: other: Maron, D.M. and Ames, B.M. (1983)
Year: 1996
GLP: no
Test substance: other TS: Tributyl phosphate, highest purity available, was provided by Tokyo Kasei

Method: Guideline Followed: None
Test Type: Microbial Mutagenicity Test
Analytical monitoring: No
Exposure Period: Varied according to organism

statistical method: Statistical significance was determined using a linear regression test.
Result: Tributyl Phosphate was consistently found to be without mutagenic activity in each of the four strains in which it was evaluated, at all of the dose levels used, with and without metabolic activation, at all of the participating facilities at which it was evaluated.
Test condition: A collaborative study was conducted in which 20 participating laboratories evaluated the mutagenic activity of 29 chemicals, including tributyl phosphate. The objective was to determine the consistency of the interlaboratory results and the sensitivity of the four bacterial strains. Tributyl phosphate was evaluated in Salmonella typhimurium strains TA102 and TA 2638 and in Escherichia coli strains WP2/pKM101 and WP2 uvrA/pKM101, using the plate incorporation method, with and without metabolic activation. The activation system was prepared from rat livers induced by phenobarbital and 5,6-benzoflavone. The plates were incubated at 37 C for 48 hours after which colonies were quantified by an automated colony counter. The test included 5 dose levels and replicates of 3 plates per dose. The doses of tributyl phosphate used in all of the tests were 5000, 2500, 2000, 1250, 1000, 625, 500, 313, 250, 125, 78, 31.3, and 0 ug/plate. Positive controls, included in each test, were mitomycin C, 2-minoanthracene, and 2-(2-furyl)-3-(5-nitro-2-furyl) acrylamide.
Conclusion: Tributyl phosphate was not mutagenic in any of the four bacterial strains in which it was tested, with or without metabolic activation.

Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
18-JUL-2005 (123)

Type: Ames test
System of testing: S. typhimurium TA1535, TA100, TA1537, TA98
Metabolic activation: with and without
Result: negative

GLP: no data
Test substance: no data

11-MAY-2005 (11)

Type: Ames test
System of testing: S. typhimurium LT-2 (hisC117, hisG46, TA1530, hisD3052, TA1531, TA1532)
Metabolic activation: without
Result: negative

GLP: no data
Test substance: no data

11-MAY-2005 (63)

Type: Ames test
System of testing: S. typhimurium TA1535, TA1538, TA1537, TA98, TA100
Metabolic activation: with and without
Result: negative

GLP: no data
Test substance: as prescribed by 1.1 - 1.4

11-MAY-2005 (52)

Type: Ames test
System of testing: S. typhimurium TA1535, TA1538
Metabolic activation: with and without
Result: positive

GLP: no data
Test substance: no data

11-MAY-2005 (61)

Type: Ames test
System of testing: no data
Metabolic activation: with and without
Result: negative

GLP: no data
Test substance: no data

11-MAY-2005 (23)

Type: Bacterial reverse mutation assay
System of testing: E. coli WP2 isogenic strains
Metabolic activation: without

Result: negative

GLP: no data
Test substance: no data

11-MAY-2005 (63)

Type: Cytogenetic assay
System of testing: chinese hamster ovary cells (CHO-K1)
Concentration: up to 0.15 ul/ml
Metabolic activation: with and without
Result: negative

GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: chromosome aberration assay
11-MAY-2005 (91)

Type: Cytogenetic assay
System of testing: mouse embryo, 48 and 144 h post conceptionem
Metabolic activation: without
Result: negative

GLP: no data
Test substance: no data

Remark: no induction of micronuclei
11-MAY-2005 (99)

Type: Mammalian cell gene mutation assay
System of testing: CHO-K1-BH4 cells
Concentration: 0.11, 0.09, 0.08, 0.07, and 0.05 ul/ml without S-9 and 0.15, 0.125, 0.1, 0.08 and 0.06 ul/ml with S-9
Metabolic activation: with and without
Result: negative

GLP: yes
Test substance: as prescribed by 1.1 - 1.4

18-JUL-2005 (90)

5.6 Genetic Toxicity 'in Vivo'

Type: Cytogenetic assay
Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: single administration
Doses: 0, 300, 600, or 1200 mg/kg bw
Result: negative

Method: other: U.S. EPA TSCA Test Guideline 798.5385
Year: 1991
GLP: yes

Test substance: other TS: Tributyl phosphate, lot number 2B-131, 99.5% pure, was provided by FMC Corporation.

Method: Test Type: In Vivo Mammalian Bone Marrow Cytogenetics: Chromosome Analysis
Species/Strain/Supplier: Sprague-Dawley Rats from Charles River Breeding Laboratories
Statistical Methods: Fisher's exact test was used to compare the percent of aberrant cells between treatment and control groups. The Cochran-Armitage test was used to evaluate dose-response.

Result: One male and four females died in the high dose group and were replaced with treated animals from a replacement group run in parallel. Clinical signs, observed in just a few animals, included diarrhea and irregular breathing. The total number of aberrations such as gaps, breaks, and abearrangements, were tabularized for each group. In addition, chromatid-type breaks and exchanges were

tabularized. The percent of chromosomal damage was not significantly increased in the tributyl phosphate treated animals, regardless of sex, dose, or sacrifice time. In contrast, the positive control chemical, cyclophosphamide, induced a significant increase in cells containing one or more aberrations. In this test, tributyl phosphate did not induce chromosomal damage in rat bone marrow cells.

Test condition: This study was conducted to determine the ability of tributyl phosphate to induce Structure chromosomal aberrations in rats after a single exposure. Fifteen males and fifteen females, about 6 to 8 weeks of age, were assigned to each of the 5 test groups. Single oral tributyl phosphate doses were 300, 600, or 1200 mg/kg. The positive control group received a single 20 mg/kg dose of cyclophosphamide. The vehicle control group received corn oil in the amount of 10 ml/kg. The animals were housed at 74+-6 degree F with relative humidity at 50+-20%. Five male and five female animals from each group were sacrificed either 12, 24, or 36 hours after dose administration. Immediately after sacrifice by carbon dioxide, the femur was exposed, and bone marrow was aspirated into a syringe. The bone marrow cells were processed and prepared on glass slides (stained with Giemsa) for microscopic examination. At least 3 slides were prepared from each animal. Slides were coded and scored "blind." A minimum of 50 metaphase cells containing 40+-2 centromeres were examined from each animal and scored for chromatid type and chromosome-type aberrations.

Conclusion: Tributyl phosphate did not induce chromosomal aberrations in this test.

Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
18-JUL-2005 (89)

Type: Drosophila SLRL test
Species: Drosophila melanogaster Sex:
Route of admin.: oral feed

GLP: no data
Test substance: no data

Remark: 11.1 % lethals; doses not mentioned.
Result: negative
11-MAY-2005 (63)

5.7 Carcinogenicity

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of administration: oral feed
Exposure period: 24 months
Doses: 200, 700 and 3000 ppm
Control Group: yes

Method: other: US EPA/TSCA Guideline No. 798.3320
Year: 1996
GLP: yes
Test substance: other TS: Tributyl phosphate, 99.7% pure, was provided by FMC Corporation.

Method: Test Type: 24-Month Oral (Dietary) Toxicity/Carcinogenicity Study in Rats
Species/Strain/Supplier: Sprague-Dawley Rats from Charles River, Kingston, NY
Analytical monitoring: yes
Statistical Methods: Bartlett's test was performed at the 1% two-sided risk level, to evaluate variance. Analysis of variance (ANOVA) was then performed, using parametric procedures in cases of unequal variance. Parametric procedures consisted of a one-way ANOVA using the F-distribution to assess significance and Dunnett's test to determine differences from control. Standard regression techniques with tests for trend and lack of fit were used to evaluate dose-related trends. Non-parametric procedures were those described by Hollander and Wolfe and consisted of the Kruskal-Wallis test for significance. Dunn's summed rank test and Jonckheere's test were also applied.
Result: Chronic exposure to tributyl phosphate did not affect survival. The primary clinical sign observed was red discoloration of the urine, in 2/50, 3/50, 3/50 and 14/50 males and 0/50, 0/50, 1/50 and 2/50 females in the 0, 200, 700, and 3000 ppm groups, respectively. The discoloration occurred most frequently between weeks 46 and 104. Food consumption was unaffected. Body weight gain in the high dose animals was significantly lower than in the corresponding control animals. Hematology and urinalysis parameters were unaffected by treatment. A dose-related increase in the incidence and severity of urinary bladder hyperplasia and the incidence of urinary bladder papillomas

was observed in both male and female animals in the mid and high dose groups. Transitional cell carcinomas of the urinary bladder were present in 6 of 49 males and in 2 of 50 females in the high dose group, and a single squamous cell carcinoma was present in 1 of the 49 high dose males. The oncogenic effects showed a clear threshold of 700 ppm in the diet. The NOEL for chronic toxicity was 200 ppm. The mean intake of tributyl phosphate for the high dose male and female animals was 143 and 182 mg/kg/day. The consistently negative mutagenicity tests indicate that the urinary bladder tumors

are induced by a nongenotoxic (epigemetic) mechanism.

Test condition: This study was conducted to determine the toxicity and carcinogenic potential of tributyl phosphate after daily exposure for 24 months. Male and female rats were 4 weeks old at receipt, and were quarantined for two weeks prior to being placed in the study. Fifty male and 50 female rats were randomly allocated to each of four groups. Tributyl phosphate was administered daily in the diet, at levels of either 200, 700, or 3000 ppm. A control group received just rodent diet. Body weights and food consumption were measured weekly for the first 13 weeks and monthly thereafter. Hematologic evaluations were performed at 12, 18, and 24 months Hematology parameters measured include hematocrit, hemoglobin, erythrocyte count, leukocytes (total and differential), platelet count, mean corpuscular volume, and prothrombin time. Urine analysis occurred at 3 weeks and at 3, 6, 12, and 18 months. All animals were euthanized after 24 months of exposure to tributyl phosphate, and underwent examination for gross lesions during necropsy.
The following tissues were taken from each animal for examination: brain, spinal cord (3 levels), pituitary, thyroid with parathyroids, thymus, trachea, lungs, heart, liver, spleen, pancreas, kidneys, adrenals, muscle, eyes, prostate, mammary gland, skin, testes, ovaries, uterus, aorta, esophagus, stomach, duodenum, jejunum, ileum, colon, rectum, urinary bladder, and sciatic nerves. All tissues were examined from the control and high dose animals. In addition, the liver, kidney, and urinary bladder were examined from all animals in the other groups. Urinary bladders were examined for the presence of calculi. If calculi were observed, the bladder was inflated with fixative and allowed to fix for five minutes prior to having the calculi removed. Any urinary calculi found at necropsy were saved and analyzed for calcium, magnesium, and phosphorus.

Conclusion: The NOAEL for chronic toxicity was 200 ppm (9mg/kg/day for males and 12 mg/kg/day for females). Chronic exposure to the highest dose, 3000 ppm, resulted in an increased incidence of transitional cell tumors of the urinary bladder. A significant increase in urinary bladder hyperplasia was observed in the mid dose animals.

Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
18-JUL-2005 (65)

Species: mouse Sex: male/female
Strain: CD-1
Route of administration: oral feed
Exposure period: 18 months
Doses: 150, 1000, 3500 ppm
Control Group: yes

Method: other: US EPA/TSCA Guideline No. 798.3300
Year: 1996
GLP: yes
Test substance: other TS: Tributyl phosphate, 99.7% pure, was provided by FMC Corporation.

Method: Test Type: 18-Month Oral (Dietary) Carcinogenicity Study in Mice
Species/Strain/Supplier: CD-1 Mice from Charles River, Kingston, NY
Analytical monitoring: yes
Statistical Methods: Bartlett's test was performed at the 1% two-sided risk level, to evaluate variance.
Analysis of variance (ANOVA) was then performed, using parametric procedures in cases of unequal variance. Parametric procedures consisted of a one-way ANOVA using the F-distribution to assess significance and Dunnett's test to determine differences from control. Standard regression techniques with tests for trend and lack of fit were used to evaluate dose-related trends. Non-parametric procedures were those described by Hollander and Wolfe and consisted of the Kruskal-Wallis test for significance. Dunn's summed rank test and Jonckheere's test were also applied.
Result: Dietary exposure for 18 months to tributyl phosphate did not affect survival. Clinical signs and hematology parameters were also unaffected by treatment.
Food consumption was unaffected. Body weight gain in the high dose animals as significantly lower than in the corresponding control animals. A significant dose-related increase in absolute and relative liver weights was observed in the mid and high dose male and female animals. The incidence of hepatocellular adenomas was significantly increased in male mice in the high dose group (3/50 in control mice vs. 10/50 in the high dose mice). Historical control data from the laboratory shows indices as high as 10 hepatocellular adenomas in 60 males, which indicates the results in this study may not be biologically significant. No other tumors were observed in any of the groups in this study. The NOEL for chronic toxicity was 150 ppm (28.9 mg/kg/day for females and 24.1 mg/kg/day for males). The mean intake of tributyl phosphate for the high dose male and female animals was 585 and 711 mg/kg/day.
Test condition: This study was conducted to determine the carcinogenic potential of tributyl phosphate after daily dietary exposure for 18 months. Male and female mice were

Species: mouse Sex: male/female
Strain: CD-1
Route of administration: oral feed
Exposure period: 18 months
Doses: 150, 1000, 3500 ppm
Control Group: yes

Method: other: US EPA/TSCA Guideline No. 798.3300
Year: 1996
GLP: yes
Test substance: other TS: Tributyl phosphate, 99.7% pure, was provided by FMC Corporation.

Method: Test Type: 18-Month Oral (Dietary) Carcinogenicity Study in Mice
Species/Strain/Supplier: CD-1 Mice from Charles River, Kingston, NY
Analytical monitoring: yes
Statistical Methods: Bartlett's test was performed at the 1% two-sided risk level, to evaluate variance.
Analysis of variance (ANOVA) was then performed, using parametric procedures in cases of unequal variance. Parametric procedures consisted of a one-way ANOVA using the F-distribution to assess significance and Dunnett's test to determine differences from control. Standard regression techniques with tests for trend and lack of fit were used to evaluate dose-related trends. Non-parametric procedures were those described by Hollander and Wolfe and consisted of the Kruskal-Wallis test for significance. Dunn's summed rank test and Jonckheere's test were also applied.
Result: Dietary exposure for 18 months to tributyl phosphate did not affect survival. Clinical signs and hematology parameters were also unaffected by treatment.
Food consumption was unaffected. Body weight gain in the high dose animals as significantly lower than in the corresponding control animals. A significant dose-related increase in absolute and relative liver weights was observed in the mid and high dose male and female animals. The incidence of hepatocellular adenomas was significantly increased in male mice in the high dose group (3/50 in control mice vs. 10/50 in the high dose mice). Historical control data from the laboratory shows indices as high as 10 hepatocellular adenomas in 60 males, which indicates the results in this study may not be biologically significant. No other tumors were observed in any of the groups in this study. The NOEL for chronic toxicity was 150 ppm (28.9 mg/kg/day for females and 24.1 mg/kg/day for males). The mean intake of tributyl phosphate for the high dose male and female animals was 585 and 711 mg/kg/day.
Test condition: This study was conducted to determine the carcinogenic potential of tributyl phosphate after daily dietary exposure for 18 months. Male and female mice were

4 weeks old at receipt, and were quarantined for two weeks prior to being placed in the study. Fifty male and 50

female mice were randomly allocated to each of four groups. Tributyl phosphate was administered daily in the diet, at levels of either 150, 1000, or 3500 ppm. A control group received just rodent diet. Body weights and food consumption were measured weekly for the first 13 weeks and monthly thereafter. Hematologic evaluations were performed at 12, and 18 months. Hematology parameters measured include hematocrit, hemoglobin, erythrocyte count, leukocytes (total and differential), and platelet count. All animals were euthanized after 18 months of dietary exposure to tributyl phosphate, and underwent examination for gross lesions during necropsy.

The following tissues were taken from each animal for examination: brain, spinal cord (3 levels), pituitary, thyroid with parathyroids, thymus, trachea, lungs, heart, liver, spleen, pancreas, kidneys, adrenals, muscle, eyes, prostate, mammary gland,, skin, testes, ovaries, uterus, aorta, esophagus, stomach, duodenum, jejunum, ileum, colon, rectum, urinary bladder, and sciatic nerves. All tissues were examined from the control and high dose animals. In addition, the liver, kidney, and urinary bladder were examined from all animals in the other groups.

Conclusion: The NOAEL for chronic toxicity was 150 ppm in the diet. Exposure for 18 months to the mid and high doses resulted in an increase in benign liver tumors.

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

29-JUL-2005 (9)

5.8.1 Toxicity to Fertility

Type:	Two generation study
Species:	rat
Sex:	male/female
Strain:	Sprague-Dawley
Route of administration:	oral feed
Frequency of treatment:	daily (feeding study)
Duration of test:	13 weeks F0 generation, 11 weeks F1 generation
Doses:	200, 700 and 3000 mg/kg diet (approx 15, 53 and 225 mg/kg bw/day)
Control Group:	yes
NOAEL Parental:	< 200 ppm
other: NOAEL reproductive toxicity :	>= 3000 ppm

Year: 1992

GLP: yes

Test substance: other TS: Tributyl phosphate, lot number 9B-125, 99.7% pure, was provided by FMC Corporation.

Method: Year: 1991-92
Species/Strain/Supplier: Sprague-Dawley Rats from Charles River Laboratories

Analytical Monitoring: Yes
Statistical Methods: Parametric and nonparametric statistical programs were applied.
Parametric evaluations include general linear models (SAS Institute Inc.), analysis of variance (ANOVA), arcsine-square root transformation, and Bartlett's test for homogeneity. Other tests employed include Dunnett's test was used to determine significant differences and the nonparametric Kruskal-Wallis test and Mann-Whitney U test for individual comparisons.

Remark: 30 animals/sex/group

Result: Adult toxicity was observed in both sexes and generations in the 700 and 3000 ppm dose groups. In the 3000 ppm group, there was no mortality and no treatment-related clinical observations in either male or female animals. Both sexes in both generations exhibited consistent reductions in body weights, weight gains, and food consumption. There were no gross lesions associated with treatment in the 3000 ppm males and females, but histologically the F0 and F1 males and females exhibited urinary bladder epithelial hyperplasia. In addition, animals from this dose group showed hepatic centrilobular hypertrophy.
There were no effects on any other organ or tissue in the high dose animals. There was no mortality or clinical observations in the 700 ppm animals. Reductions in body weights and weight gains were observed only in the F1 females. There were no gross findings at necropsy. Histologically, the 700 ppm male and female F0 and F1 animals showed urinary bladder hyperplasia, and the females of both generations displayed hepatic centrilobular hypertrophy. The 200 ppm also displayed urinary bladder hyperplasia but the hepatic changes observed in the animals that received the higher doses were absent in these animals. There were no effects on reproductive parameters at any dose level in either the F0 or F1 generations, including mating and fertility indices, and length of gestation. There were no treatment-related lesions in the reproductive organs of the F0 and F1 male and female animals at any dose level. Further, there were no treatment-related effects at any dose level on any parameter measured in the offspring, including litter size, sex ratio, and pre- or postnatal loss. F0 and F1 pup body weights were consistently and significantly reduced in the 3000 ppm offspring. Occasional body weight reductions were observed in the 700 ppm pups. A no observable adverse effect level (NOAEL) for adult toxicity could not be established. However, an NOAEL for reproductive toxicity was at least 3000 ppm. The results of this study confirm that tributyl phosphate is not a reproductive toxicant.

Test condition: This study was conducted to determine the effects of repeated exposure to tributyl phosphate on reproduction and fertility. The animals were 7 weeks old upon arrival and were held for a one week quarantine before being incorporated in the study. Thirty weanling rats per sex per dose (the F0 generation) were administered tributyl

phosphate in the diet for 10 weeks. Dietary concentrations were 0, 200, 700, and 3000 ppm. The animals were observed daily for clinical signs and mortality. Body weights and food consumption were measured weekly.
At the 10 weeks of exposure, each female was mated with a single male from the same dose group for 3 weeks, with continued dietary exposure to tributyl phosphate. Observations of vaginal sperm and/or copulation plugs were considered evidence of a successful mating. The dat of insemination was identified as gestation day 0. Dams were weighed and food consumption recorded on gestation days 0, 7, 14, and 20. Exposure was continued through gestation and weaning. The date of parturition was designated postnatal day 0. Pups were individually counted, examined, and sexed and were weighed individually on postnatal days 1, 4, 7, 14, and 21. At weaning, 30 F1 weanlings /sex/dose group were randomly selected to be parents of the F2 generation. Ten F1 pups/sex/group were randomly selected for necropsy. The selected F1 weanlings were exposed via the diet to the same doses of tributyl phosphate for 11 weeks and them mated. The F1 dams and F2 liters were handled as described above for the F0 dams and F1 offspring.

F0 and F1 animals underwent necropsy, gross examination, with retention of the following organs: pituitary, ovaries, testes, vagina, uterus, epididymides, seminal vesicles, prostate, urinary bladder, kidneys, and liver. All of the listed tissues from the high dose and control animals were processed through histology and examined microscopically for treatment-related changes. In addition, the kidneys, livers, and urinary bladders were examined from all the animals in all dose groups.

Conclusion: Tributyl phosphate did not cause reproductive toxicity or adversely affect fertility in this study.

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

29-JUL-2005 (104)

5.8.2 Developmental Toxicity/Teratogenicity

Species: rat Sex: female

Strain: Sprague-Dawley
Route of administration: gavage
Exposure period: day 6 to 15 of gestation
Frequency of treatment: daily
Duration of test: up to day 20 of gestation
Doses: 80, 435, 790, 1145, and 1500 mg/kg bw
Control Group: yes

GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: range-finding study, 5 animals/group
Result: considerable maternal mortility at dose levels of 790, 1145 and 1500 mg/kg bw. A dose of 80 mg/kg bw was not considered to be maternally toxic, embryotoxic or fetotoxic.
At 435 mg/kg bw maternal toxicity but no effect on embryo.
11-MAY-2005 (17)

Species: rat Sex: female
Strain: Wistar
Route of administration: gavage
Exposure period: day 7 to 17 of gestation
Frequency of treatment: daily
Duration of test: day 20 of gestation
Doses: 62.5, 125, 250 or 500 mg/kg/day
Control Group: yes
NOAEL Maternal Toxity: = 62.5 mg/kg bw
NOAEL Teratogenicity: > 250 mg/kg bw

GLP: no data
Test substance: no data

Remark: 20 animals/group
Result: Salivation and depression of body weight gain, adjusted body weight gain and food consumption were observed at the higher doses. There were no significant differences between the groups in the incidence of dead or resorbed fetuses, the number of living fetuses and the body weights of living fetuses of both sexes. The incidence of rudimentary lumbar rib was increased significantly at 500 mg/kg/day. There was one incident of conjoined twins exhibiting three fore-limbs and four hind-limbs at 125 mg/kg/day. This malformation is rare in the background data of teratology , and the incidence of malformed fetuses was not increased significantly. Therefore, TBP was considered not to be teratogenic in this study.
18-JUL-2005 (100)

Species: rabbit Sex: female
Strain: other: New Zealand
Route of administration: gavage
Exposure period: day 6 to 18 of gestation
Frequency of treatment: daily
Duration of test: up to day 30 of gestation
Doses: 50, 150 or 400 mg/kg bw

Control Group: yes
NOAEL Teratogenicity: > 400 mg/kg bw

GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: 18 animals/group
Result: at the 400 mg/kg/day dose level maternal toxic effect (mean weight loss) and not statistically significant increase of resorptions, no fetotoxic or teratogenic effects, at the 50 and 150 mg/kg/day dose level no maternal toxicity, no embryotoxic, fetotoxic or teratogenic effects.

11-MAY-2005 (20)

Species: rabbit Sex: female
Strain: other: New Zealand
Route of administration: gavage
Exposure period: day 6 to 18 of gestation
Frequency of treatment: daily
Duration of test: up to day 30 of gestation
Doses: 50, 250, 412, 775, 1137 and 1500 mg/kg bw
Control Group: yes

GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: range-finding study, 5 animals/group
Result: all animal in the 775, 1137 and 1500 mg groups died during treatment, with 250 and 412 mg/kg maternal mortality 20 %, at 50 mg/kg bw no maternal toxicity. No fetotoxicity was evident in the 50, 250 or 412 mg group, no teratogenicity.

11-MAY-2005 (19)

Species: hen Sex: no data
Strain: no data
Route of administration: other
Exposure period: single injection in the jolk sac
Doses: 5 mg/egg
Control Group: yes

GLP: no data
Test substance: no data

Remark: post obs. period: 17 days

purity not mentioned
Result: weak effects (decrease of survival, weight and length)
11-MAY-2005 (105)

Species: rat Sex: female
Strain: Sprague-Dawley
Route of administration: gavage
Exposure period: day 6 to 15 of gestation
Frequency of treatment: daily
Duration of test: up to day 20 of gestation
Doses: 188, 375, or 750 mg/kg bw
Control Group: yes
NOAEL Maternal Toxity: < 188 mg/kg bw
NOAEL Teratogenicity: > 750 mg/kg bw

Year: 1991
GLP: yes
Test substance: other TS: Tributyl phosphate, lot number 9B-125, 99.7% pure, was provided by FMC Corporation.

Method: Test Type: Developmental Toxicity Study
Year: 1990-91
Species/Strain/Supplier: Sprague-Dawley Rats from Charles River Laboratories
Analytical Monitoring: Yes
Statistical Methods: The following statistical methods were used to identify significant differences: Chi-square analysis of Snedecor and Cochran, Fisher Exact Test, Bonferroni Inequality Test, and Armitage's Test.
Remark: 24 animals/group
Result: Pregnancy rates for the control, low, mid, and high dose animals were 95.7%, 100%, 95.8%, and 95.8%, respectively. Food consumption was not reduced in the low dose group but was reduced in the mid and high dose groups. There was no effect on mean number of corpora lutea, number of pups per litter, or mean number of resorptions sites per pregnant female. Dams that received 750 mg/kg/day exhibited serious maternal toxicity, expressed as significant mortality (7 of 24 females died, 29.2%) and lower mean body weights on days 9, 12, 16, and 20, during which time the animals actually lost weight. While there was no embryotoxicity in the pups of this group, there was a significant reduction in mean fetal weight. The relative liver weight in these animals was significantly higher than control relative weights when compared to the

respective body weights. Dams in the 188
and 375 mg/kg/day groups showed reduced body weights at gestation days 16 and 20, and a reduction in weight gain during days 1-16, but there was no mortality in these groups. No embryotoxicity was observed in the pups from the 188 and 375 mg/kg/day dams. The number of fetuses with visceral malformations for the control, low, mid, and high dose groups were 0.6% (1/181 fetuses), 0.5% (1/193 fetuses), 1.1% (2/189 fetuses) and 0.7% 1/134 fetuses). The incidence of skeletal malformations for these groups were 0% (168 fetuses) evaluated), 0.06% (1/177 fetuses), 0% (0/173 fetuses), and 1.6% (2/124 fetuses), respectively. The incidence on a per fetus or per liter basis did not differ significantly between treated and control groups.
External, visceral, and skeletal examination of the fetuses

recovered from female rats in the treated groups on gestation day 20 revealed no teratogenic response at any of the dose levels evaluated in this study.

Test condition: This study was conducted to determine the effects of repeated exposure to tributyl phosphate on the pregnant rat and the developing fetuses. Tributyl phosphate was administered daily by oral gavage to 24 pregnant female rats per group, during gestation days 6-15. Dosing solutions were prepared fresh weekly and were analyzed to confirm cocentration. Dose levels were 188, 375, and 750 mg/kg/day. Since the test substance was diluted with corn oil for dosing, a corn oil control group was included in the study. The animals were observed twice daily for mortality and morbidity, and for clinical signs of toxicity. The pregnant animals were weighed on days 0, 6, 9, 12, 16, and 20 of gestation and food consumption was determined for days 0-6, 6-11, 11-16, and 16-20 of gestation. The dams were sacrificed on gestation day 20 and subjected to gross examination. The liver and gravid uterus from each animal were weighed. The number of fetuses and resorptions sites were determined. The ovaries were removed and the number of corpora lutea per ovary was recorded. The fetuses were removed, sexed, weighed, and examined for external malformations. Litter size was documented. One-half of the fetuses in each litter were processed for visceral evaluation, using the Staples' micro-dissection procedure. The remaining fetuses were stained with Alizarin Red S and evaluated for skeletal malformations and ossification variations.

Conclusion: Tributyl phosphate was maternally toxic at all 3 dose levels but did not cause a teratogenic response in the fetuses of any treatment group in this study.

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

18-JUL-2005 (18)

5.8.3 Toxicity to Reproduction, Other Studies

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5.9 Specific Investigations

Endpoint:	Neurotoxicity
Type:	other: 13 Week Oral (Gavage) Study in Rats
Species:	rat
Strain:	Sprague-Dawley Sex: male/female
Route of administration:	oral (gavage)
No. of animals:	24
Vehicle:	other: corn oil
Exposure Period:	91 day(s)
Doses:	32.5, 100 or 325 mg/kg/day
Control Group:	yes, concurrent vehicle

Method: other: U.S. EPA TSCA Subchronic Neurotoxicity Screening Battery, as identified in Subpart G, Guidelines 798.6050, 798.6200, and 798.6400

Year: 1991

GLP: yes

Test substance: other TS: Tributyl phosphate, lot number 92B-125, was provided

by FMC Corporation

Method: Statistical Methods: Group variances for body weight, food consumption, grip strength, hindlimb splay, and brain measurements were tested using Bartlett's test.
Since differences between group variances were not significant, a one-way analysis of variance (ANOVA) was performed. Dunnett's test was used to compare the control and treated groups.

Remark: This study was conducted to assess the potential neurotoxicity of tributyl phosphate using a functional observation battery, motor activity battery, and a neuropathological examination. Body weights and food consumption were measured weekly. Twelve male and 12 female rats were randomly allocated to each of four groups.
Tributyl phosphate was administered daily by oral gavage at doses of 32.5, 100, or 325 mg/kg/day. A control group received just corn oil (vehicle). The animals were evaluated with a functional observation battery prior to the first dose, at 1, 6, and 12 hours after the first dose, and prior to dosing on days 7, 14, 35, 63, and 91. Motor activity evaluations were performed prior to the first dose and on study days 28, 62, and 90. At the completion of the in-life phase of the study, 6 animals per sex per group were randomly selected for perfusion and neuropathological evaluation. Neurological tissues examined include forebrain, midbrain, cerebellum, medulla oblongata, pons, cervical and lumbar spinal cord, sural nerve, tibial nerve, and certain ganglia. Many other tissues were collected from each animal and preserved for possible future examination. During the study, all animals were observed daily for appearance, behavior, and mortality.

Result: Two males and 1 female in the mid-dose group and 3 males and 4 females in the high dose group died during the study. Male and female rats in the high dose group showed a higher incidence of muzzle staining, urogenital staining, and

alopecia on their limbs and body. Body weight loss was observed in the males (beginning on day 14) and females (beginning on day 35) of the high dose group.
Body weights of the mid and low dose animals were comparable to that of the control animals. A significant decrease in food consumption was seen only in the high dose animals during the first week of dosing.

Qualitative functional observation battery evaluations (body position, locomotor activity, bizarre behavior, tremors, etc.) and quantitative functional observation battery measurements (grip strength, hind limb splay, etc.) did not reveal any treatment-related differences. There were no significant differences in motor activity test results between the treated and control animals. Microscopic examination of the nervous system did not find any treatment-related neuropathology. Brain weight, length, and width measurements showed no treatment-related differences.

Conclusion: The NOAEL for male and female rats is greater than 325 mg/kg/day, the highest dose administered in this study.

Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint

18-JUL-2005 (15)

5.10 Exposure Experience

Remark: some decrease in nonspecific esterase straining of monocytes in occupational exposed persons.
18-JUL-2005 (85)

Remark: skin pentration in vivo and in vitro: maximum steady state penetration rate 0.18 ug/cm3/min.
18-JUL-2005 (86)

Remark: workers exposed to 15 mg/m3 of tributyl phosphate have complained of nausea and headache
18-JUL-2005 (87)

Remark: irritant effect on skin and mucous membranes (no further data).
18-JUL-2005 (7) (116)

Remark: an abstract of a Soviet paper states that exposure to unspecified quantities during the production of scandium oxide may have been responsible (together with other compounds) for skin rashes in workers (no further information)
18-JUL-2005 (49)

5.11 Additional Remarks

Type: Cytotoxicity

Remark: Cytotoxicity in vitro: tributyl phosphate inactivate lipid-enveloped viruses, but did not alter the function of serum proteins.

11-MAY-2005 (36)

Type: Cytotoxicity

Remark: Cytotoxic effects in vitro (HeLa cells)

11-MAY-2005 (43)

Type: Metabolism

Remark: rat, single i.p. injection of 1 mmol: decrease of glutathione in liver and kidney; small amounts of oxidized butyl moieties were removed as glutathione conjugates and excreted as S-containing metabolites in urine: (3-oxobutyl)- and (3-hydroxybutyl)mercapturic acids (8.9 and 5.2 % of applied dose), other S-butylmercapturic acid derivatives were found only in traces. After i.p. injection of the probable intermediate dibutyl-hydrogenphosphate, only 0.07 and 0.02 % of the

applied dose was eliminated as S-containing metabolites in the urine.

11-MAY-2005 (117)

Type: Metabolism

Remark: (14C-labelled substance was used):
- rat, oral: 14 mg/kg: within 1 day, 50 % were excreted in urine, 10 % in exhaled air and 6 % in feces; total elimination after 5 days 82 %
- rat, i.p.: 14 mg/kg: within 1 day, 70 % were excreted with urine, 7 % with exhaled air and 4 % in feces; total elimination after 5 days 90 %.
- rat, i.p.: 250 mg/kg: 11 phosphorous-containing metabolites in 24-h urine were identified in the neutral and actid fractions with atotal recovery of 25 and 12 %. Major metabolites: dibutylhydrogen phosphate(40-64 % of identified dose), butyl dihydrogen phosphate(11-21 % of identified dose), butyl bis (3-hydroxybutyl) phosphate (3-4 % of identified dose) and small amounts of derivatives hydroxylated at the butyl moieties.
1 unidentified neutral metabolite was shown in the gas chromatogram. The butanol-extractable metabolites (25 % of the dose), which were not quantitated, were butyl-3-hydroxybutylphosphat, 3-hydroxybutylphosphat and monobutylphosphat.
47.6 % of dibutyl hydrogenphosphate recovered intact in

urine after i.p. infection, therefore the authors concluded that dibutyl hydrogen phosphate produced as an intermediate in the metabolism of tributylphosphate would be mostly excreted. The data after administration of probable metabolic intermediate suggest, that hydroxylation at C-3 is an early metabolic process, which is followed by further metabolic reactions (oxidation to produce carboxylic acids and ketones). The oxo compound (dibutyl 3-oxobutyl phosphate) dibutyl hydrogen phosphate.

11-MAY-2005 (118)

Type: Metabolism

Remark: cholinesterase inhibition: rat, i.p., 16-266 mg/kg bw (0.062-1 mmole/kg): 21 % inhibition of cholinesterase, increased activity of beta-glucuronidase in plasma.

11-MAY-2005 (119)

Type: Metabolism

Remark: skin of living pigs: hair follicle is not more penetrable than other dermal area; in fact, regions of the skin devoid of follicules were penetrated slightly more rapidly than areas containing follicles.

11-MAY-2005 (78)

Type: Metabolism

Remark: following single or repeated oral dosing in rats, tributyl phosphate was detected in the gastrointestinal tract, blood and liver (no further data).

11-MAY-2005 (75)

Type: Metabolism

Remark: tributyl phosphate is metabolized in rodents to butyl-n-cysteine (no further data).

11-MAY-2005 (71)

Type: Metabolism

Remark: in vitro: rat liver homogenate: rapid metabolism in the presence of NADPH, but only slight breakdown in the absence of added NADPH. Dibutyl(3-hydroxybutyl)phosphate was obtained as a metabolite in the first stage. The extended incubation time yielded two metabolites: butyl di(3-hydroxy- butyl)phosohate and dibutyl hydrogen phosphate.

11-MAY-2005 (112)

Type: Metabolism

Remark: (14C labelled tributyl phosphate was used):
rat, single i.v. injection of 5 mg/kg;
rat, single dermal application of 10 or 350 mg/kg;
rat, single oral dose of 10 and 350 mg/kg;
rat, multiple oral dose (8x) of 10 or 350 mg/kg:
no adverse signs of toxicity in any low dose group, in all high dose groups red urine and/or hypersalivation, blood in urine in all dose groups. The major proportion of the recoverable radioactivity was eliminated within 48 h in urine and feces. The major route of elimination is via the kidneys (65-85 % of dose after oral and i.v. application). The distribution pattern in the tissues was similiar in all dose groups. The HPLC analysis showed 9 major and 6 minor regions of radioactivity in the urine, mass spectrometric analyses revealed monobutylphosphate, dibutylphosphate, butyl-2-hydroxybutyl phosphate and 3-carboxypropyl-dimethylphosphate. The author concluded, that the butyl groups of tributylphosphate are oxidized to alcoholic, ketonic and acific functionalities. The oxidized chains are also hydrolysed proceeding to the di-, mono- and the unsubstituted phosphoric acids.

11-MAY-2005 (92)

Type: Neurotoxicity

Remark: hen, oral, two doses of 1500 mg/kg bw (LD50) 21 days apart, killed 21 days after the second dose: no nerve damage or clinical signs of toxicity (purity of test material 98.37%).
--neurotoxicity: hen, single oral dose of 1500 mg/kg bw:

no relevant inhibition of brain NTE (neurotoxic esterase) or brain actylcholinesterase, increase of plasma cholinesterase (purity of test material 98.37%).

11-MAY-2005 (33)

Type: Neurotoxicity

Remark: hen, oral: 1840 mg/kg bw on two days: neither behavioral nor histological evidence of neurotoxicity (no further data).

18-JUL-2005 (70)

Type: Neurotoxicity

Remark: cholinesterase activity in brain and liver homogenates and serum (rat) after incubation with tributyl phosphate (purity > 97 %): no change of enzyme acitivty

18-JUL-2005 (102)

Type: Neurotoxicity

Remark: adult hen, oral or dermal 1500 mg/kg bw at day 0 and 21, observation up to day 42: no signs of neurotoxicity (purity not given).

18-JUL-2005 (95)

Type: Neurotoxicity

Remark: rat, rabbit: in lethal doses, oral or i.p., decrease of cholinesterase activity in serum, red blood cells, liver and brain of maximum 35 %.

18-JUL-2005 (73)

Type: Neurotoxicity

Remark: anticholinesterase activity in vitro, human red cell hermolysate or humanplasma: slight decrease of cholinesterase activity (purity not mentioned).

11-MAY-2005 (107)

Type: Neurotoxicity

Remark: range-finding study on motor activity in rats: single oral application of 1000 mg/kg bw, after 0.5 h following dosing, motor activity was tested for 23 hours: one treated female was found dead after 2 days, all treated animals show clinical signs of toxicity, reduced motor activity levels.

4/sex/group
purity not known

11-MAY-2005 (14)

Type: Neurotoxicity

Remark: Neurotoxicity (acute delayed) Hens, single oral dose of 1500 mg/kg with atropine protection. Second TBP dose on day 21. Cholinergic signs including salivation, miosis, and diarrhea. 4 of 20 hens died week 1 and 2, more died on week 2. No ataxia or paralysis. No histopathological lesions.

11-MAY-2005 (33)

Type: Neurotoxicity

Remark: Chicken, single 1.84 g/kg oral dose. Repeated dosing at day 21. No signs of neurotoxicity based on locomotor and neuropathology examination.
Result: Not neurotoxic

11-MAY-2005 (67)

Type: Toxicokinetics

Remark: iv (5 mg/kg); dermal (10 and 350 mg/kg - 6 hr. exposure)
Result: Minipig - iv - rapidly eliminated; dermal - poorly absorbed (1-4% excreted); no bioaccumulation in bladder or kidney; metabolism is hydroxylation followed by Phase II (glucuronide, sulfate formation).

11-MAY-2005 (88)

Type: other: Neurotoxic esterase

Remark: Hens, single dose of 1500 mg/kg. No significant change in brain neurotoxic esterase or acetylcholine esterase activity.

11-MAY-2005

Type: other: Neurotoxicity (acute delayed)

Remark: Hens, dermal exposure 1500 mg/kg day 0-21. No signs of neurotoxicity. No atropine protection.

11-MAY-2005 (33)

Type: other: other: Neurotoxicity, acute

Remark: Rats, doses of 100, 325 and 1000 mg/kg oral. Motor activity and functional observation battery.
Result: Not neurotoxic.

11-MAY-2005 (64)

Type: other: Subchronic Dietary Mechanistic Study

Result: TBP at doses of 700 and 3000 ppm appears to produce urothelial cytotoxicy with marked regenerative hyperplasia. No changes were noted on urinary parameters, other than a slight decrease in osmolality and creatinine at 3000 ppm. Effects were reversible upon withdrawal of treatment during a 10-week recovery period. The toxicity is likely due to the chemical or metabolites, not to urinary changes. A NOEL of 200 ppm was established for all parameters.

Test condition: The dose response of TBP effects on the urinary bladder and on urinary parameters was evaluated in male Sprague-Dawley rats fed 0, 200, 700 and 3000 ppm in the diet. Ten rats per

group were exposed for 10 weeks. Another group received 3000 ppm TBP plus 12,300 ppm NH4Cl. A high dose recovery group (3000 ppm TBP for 10 wks, then 10 wks control diet) was included to evaluate reversibility.

11-MAY-2005 (8)

Remark: rabbit, i.p.:100 mg/kg bw single injection: no effect
200 mg/kg bw single injection: lethal after 11 days
rabbit, s.c.: 100 or 200 mg/kg bw: no systemic effects, local inflammatory effects.

11-MAY-2005 (66)

Remark: no marked difference of LD50 values observed with oral, s.c. or i.p. administration.

11-MAY-2005 (93)

Remark: rat, single oral, i.p. or i.m. application of 0.1 to 0.2 ml: labored breathing, hypersalivation, pallor; paralysis after parenteral application; no symptoms after dermal application (purity not mentioned).

11-MAY-2005 (107)

Remark: mice, i.p., 850 - 1000 mg/kg bw: narcosis, muscular paralysis

11-MAY-2005 (35)

Remark: Reviews:
- Environmental Health Criteria 112, World Health Organization (1991)
- BIBRA Toxicity Profile (1991)
- Berufsgenossenschaft der chemischen Industrie. Toxikologische Bewertung Ausgabe 02/89, Nr. 170 (1989)

11-MAY-2005

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Remark: mice, i.p., 850 - 1000 mg/kg bw: narcosis, muscular paralysis

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Remark: Reviews:
- Environmental Health Criteria 112, World Health Organization (1991)
- BIBRA Toxicity Profile (1991)
- Berufsgenossenschaft der chemischen Industrie. Toxikologische Bewertung Ausgabe 02/89, Nr. 170 (1989)

11-MAY-2005

Remark: rat: eye and nasal irritation after 1 hour exposure to atmospheric concentrations of 200 mg/l.

11-MAY-2005 (51)

6.1 Analytical Methods

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6.2 Detection and Identification

-

7.1 Function
-

7.2 Effects on Organisms to be Controlled
-

7.3 Organisms to be Protected
-

7.4 User
-

7.5 Resistance
-

8.1 Methods Handling and Storing
-

8.2 Fire Guidance
-

8.3 Emergency Measures
-

8.4 Possib. of Rendering Subst. Harmless
-

8.5 Waste Management
-

8.6 Side-effects Detection
-

8.7 Substance Registered as Dangerous for Ground Water
-

8.8 Reactivity Towards Container Material
-

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10.1 End Point Summary

-

10.2 Hazard Summary

-

10.3 Risk Assessment

-

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I U C L I D

D a t a S e t

Existing Chemical	ID: 126-71-6
CAS No.	126-71-6
EINECS Name	triisobutyl phosphate
EC No.	204-798-3
Molecular Weight	266.32
Molecular Formula	C12H27O4P

Producer Related Part
Company: EUROPEAN COMMISSION - European Chemicals Bureau
Creation date: 11-FEB-2000

Substance Related Part
Company: EUROPEAN COMMISSION - European Chemicals Bureau
Creation date: 11-FEB-2000

Printing date:	30-JUN-2005
Revision date:	11-FEB-2000
Date of last Update:	11-FEB-2000

Number of Pages: 61

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 Applicant and Company Information
-

1.0.2 Location of Production Site, Importer or Formulator
-

1.0.3 Identity of Recipients
-

1.0.4 Details on Category/Template
-

1.1.0 Substance Identification
-

1.1.1 General Substance Information

Substance type: organic
Physical status: liquid

1.1.2 Spectra
-

1.2 Synonyms and Tradenames

Isobutyl phosphate ((C4H90)3PO) (6CI, 7CI)

Source: BASF AG Ludwigshafen

Phosphoric acid, triisobutyl ester (8CI)

Source: BASF AG Ludwigshafen

Phosphoric acid, tris(2-methylpropyl) ester (9CI)

Source: BASF AG Ludwigshafen

Phosphorsäuretriisobutylester

Source: TRANSOL Chemiehandel GmbH Essen

Triisobutyl phosphate

Source: BASF AG Ludwigshafen

1.3 Impurities
-

1.4 Additives
-

1.5 Total Quantity
-

1.6.1 Labelling

-

1.6.2 Classification
-

1.6.3 Packaging
-

1.7 Use Pattern
-

1.7.1 Detailed Use Pattern
-

1.7.2 Methods of Manufacture
-

1.8 Regulatory Measures
-

1.8.1 Occupational Exposure Limit Values

Type of limit: MAK (DE)

Remark: kein MAK-Wert festgelegt.
Source: BASF AG Ludwigshafen

(1)

Type of limit: MAK (DE)

Remark: kein MAK-Wert festgelegt.
Source: BASF AG Ludwigshafen

(2)

1.8.2 Acceptable Residues Levels
-

1.8.3 Water Pollution

Classified by: other: BASF-Selbsteinstufung
Class of danger: 1 (weakly water polluting)

Country: Deutschland
Source: BASF AG Ludwigshafen

(3)

Classified by: other: Selbsteinstufung BASF AG
Class of danger: 1 (weakly water polluting)

Source: BASF AG Ludwigshafen

(4)

1.8.4 Major Accident Hazards

Legislation: Stoerfallverordnung (DE)
Substance listed: no

Source: BASF AG Ludwigshafen

(5)

1.8.5 Air Pollution

Remark: bisher keine Zuordnung
Source: BASF AG Ludwigshafen

1.8.6 Listings e.g. Chemical Inventories
-

1.9.1 Degradation/Transformation Products
-

1.9.2 Components
-

1.10 Source of Exposure
-

1.11 Additional Remarks
-

1.12 Last Literature Search
-

1.13 Reviews
-

2.1 Melting Point

Remark: Erstarrungstemperatur: < -50 Grad C
Source: BASF AG Ludwigshafen

(6)

Remark: Erstarrungstemperatur: < -60 Grad C
Source: BASF AG Ludwigshafen

(7)

2.2 Boiling Point

Value: = 115 degree C at 30 hPa

Source: BASF AG Ludwigshafen

(8)

Value: = 115 degree C at 30 hPa

Source: BASF AG Ludwigshafen (9)

Value: = 272 degree C

Source: BASF AG Ludwigshafen (6)

Value: = 272 degree C

Source: BASF AG Ludwigshafen (7)

2.3 Density

Type: density
Value: = .96 - .965 g/cm? at 20 degree C

Source: BASF AG Ludwigshafen (6)

Type: density
Value: = .96 - .965 g/cm? at 20 degree C

Source: BASF AG Ludwigshafen (7)

Type: density
Value: = .964 g/cm? at 20 degree C

Source: BASF AG Ludwigshafen (8)

Type: density
Value: = .964 g/cm? at 20 degree C

Source: BASF AG Ludwigshafen (9)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: = 2 hPa at 103 degree C

Source: BASF AG Ludwigshafen (10)

Value: = 10 hPa at 133 degree C

Source: BASF AG Ludwigshafen (10)

Value: = 50 hPa at 170 degree C

Source: BASF AG Ludwigshafen (10)

Value: = 130 hPa at 200 degree C

Source: BASF AG Ludwigshafen (6)

Method: other (measured): dynamisch unter Argonatmosphäre
Year: 1989
GLP: no

Remark: 1013.25 hPa bei 272.46 Grad C (berechnet aus gemessenen Werten durch Regression)
Result: Temperatur in Grad C/Dampfdruck in hPa (gemessen): 91.74/1.00; 102.76/2.00; 118.94/5.00; 132.59/10.00; 169.85/50.00; 188.93/100.00; 243.2/500.0;
Source: BASF AG Ludwigshafen
Test substance: Reinheit: 98.34%
Reliability: (2) valid with restrictions
nachvollziehbar und akzeptabel (11)

2.5 Partition Coefficient

log Pow: = 3.72 at 25 degree C

Method: other (measured)

Source: BASF AG Ludwigshafen

(12)

log Pow: = 3.72 at 25 degree C

Method: other (measured)
Year: 1990
GLP: no

Source: BASF AG Ludwigshafen
Test substance: Reinheit: 98.1% (lt. GC)
Reliability: (2) valid with restrictions
nachvollziehbar und akzeptabel

(13)

2.6.1 Solubility in different media

Value: = 265 mg/l at 25 degree C

Source: BASF AG Ludwigshafen

(12)

---

pH value: = 8.5
Conc.: 100 g/l at 20 degree C

Remark: Loeslichkeit in anderen Loesemitteln: Ethanol, Glykolen, aromatische Kohlenwasserstoffe
nicht mischbar
Source: BASF AG Ludwigshafen

(6)

Remark: Reinheit: 98.1%
Die Prüfsubstanz ist hydrolysebeständig
Source: BASF AG Ludwigshafen

(14)

Value: = 265 mg/l at 25 degree C

Method: other: gaschromatographisch
Year: 1990
GLP: no

Source: BASF AG Ludwigshafen
Test substance: Reinheit: 98.1% (lt. GC)
Reliability: (2) valid with restrictions
nachvollziehbar und akzeptabel

(13)

Value: = 264 mg/l at 25 degree C
pH value: = 8.5
Conc.: 100 g/l at 20 degree C

Source: BASF AG Ludwigshafen

(7)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: = 133 degree C

Method: other: DIN 51 758

Source: BASF AG Ludwigshafen

(6)

Value: = 133 degree C

Method: other: DIN 51 758

Source: BASF AG Ludwigshafen

(7)

2.8 Auto Flammability

Value:

Remark: Zuendtemperatur: 430 Grad C (DIN 51 794)
Source: BASF AG Ludwigshafen

(6)

Value:

Remark: Zuendtemperatur: 430 Grad C (DIN 51 794)
Source: BASF AG Ludwigshafen

(7)

2.9 Flammability
-

2.10 Explosive Properties

Result: not explosive

Source: BASF AG Ludwigshafen

(6)

Result: not explosive

Source: BASF AG Ludwigshafen

(7)

2.11 Oxidizing Properties
-

2.12 Dissociation Constant
-

2.13 Viscosity
-

2.14 Additional Remarks

Result: Viskosität: 3.0 mPa*s bei 40 Grad C
2.0 mPa*s bei 60 Grad C
1.44 mPa*s bei 80 Grad C
Source: BASF AG Ludwigshafen

(9)

Result: Viskosität: ca. 20 mPa*s bei 20 Grad C (Brookfield/20 min)
Source: BASF AG Ludwigshafen

(7)

Remark: wasserdampfflüchtig
Source: BASF AG Ludwigshafen

(7)

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 500000 molecule/cm?
Rate constant: = .0000000000906808 cm^3/(molecule * sec)
Degradation: = 50 % after 4.3 hour(s)

Method: other (calculated): AOP, Version 1.51
Year: 1994
GLP: no

Source: BASF AG Ludwigshafen

(15)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 500000 molecule/cm?
Rate constant: = .0000000000906808 cm^3/(molecule * sec)
Degradation: = 50 % after 4.3 hour(s)

Method: other (calculated): AOP, Version 1.51
Year: 1994
GLP: no

Source: BASF AG Ludwigshafen

(16)

3.1.2 Stability in Water

Type: abiotic
t1/2 pH4: ca. 170 day(s) at 50 degree C
t1/2 pH7: ca. 303 day(s) at 50 degree C

Year: 1990
Test substance: other TS: Etingal

Remark: Die Substanz ist hydrolysebeständig.
Source: BASF AG Ludwigshafen

(17)

Remark: no data are available
Source: BASF AG Ludwigshafen

3.1.3 Stability in Soil

Remark: no data are available
Source: BASF AG Ludwigshafen

3.2.1 Monitoring Data (Environment)

Type of measurement: background concentration
Medium: ground water

Result: Triisobutylphosphat: highest concentration of 10 ug/l detected in the netherlands (minimum concentration less than 0.1 ug/l).
Source: BASF AG Ludwigshafen

(18)

Type of measurement: background concentration
Medium: ground water

Result: Triisobutylphosphat: highest concentration of 10 ug/l detected in the netherlands (minimum concentration less than 0.1 ug/l).
Source: BASF AG Ludwigshafen

(19)

Type of measurement: other: GC/MS (XAD)
Medium: surface water

Result: Rhine water (Netherlands))
Maassluis (07/02/78): 1 ug/l
Lobith (20/06/78): 0,3 ug/l
Source: BASF AG Ludwigshafen

(20)

Type of measurement: other: GC/MS; HPLC
Medium: surface water

Result: Triisobutylphosphat has been identified in Rhine water at several locations in the Netherlands delta: (in ug/l) Markermeer (24/01/91): 0 ; Kampen (21/04/89): 0,069; Lobith (17/03/89): 0,198; Lobith (15/09/89): 0,071; Werkendam (29/09/89): 0,08; Maassluis (26/05/89): 0,096; Maassluis (22/09/89): 0,049; Haringvliet (19/05/89): 0,05
Source: BASF AG Ludwigshafen

(21)

Type of measurement: other: GC/MS; HPLC
Medium: surface water

Result: Triisobutylphosphat has been identified in Rhine water at several locations in the Netherlands delta: (in ug/l) Markermeer (24/01/91): 0 ; Kampen (21/04/89): 0,069; Lobith (17/03/89): 0,198; Lobith (15/09/89): 0,071; Werkendam (29/09/89): 0,08; Maassluis (26/05/89): 0,096; Maassluis (22/09/89): 0,049; Haringvliet (19/05/89): 0,05
Source: BASF AG Ludwigshafen

(22)

Type of measurement: other
Medium: other: Abwasser

Remark: Untersuchungsort: Unterweser im bremischen Raum (Klaeranlagen Seehausen, Delmenhorst, Osterholz, Farge, Bremerhaven, Bremer Wollkaemmerei, Kloeckner Werke) Analysenmethode: Extraktion mit n-Hexan/Dichlormethan, GC-PND mit 2 Kapillarsaeulen
Result: mittlere Konzentration im Abwasser: ca. 500 ng/l Einzelwerte (in ng/l): Klaeranlagen Seehausen: 551-8070; Delmenhorst: 110-13600; Osterholz: 310-2610; Farge: 680-3000; Bremer Wollkaemmerei: 761-4400; Kloeckner Werke: 450-1340
Source: BASF AG Ludwigshafen

(23)

Type of measurement: other
Medium: surface water

Remark: sampling area: Llobregat River (Station A); Ebro River mouth (Station B) in Spain
sampling time: march to june 1988
sample preparation: extraction with methylene chloride
Analytical method: GC-NPD (= nitrogen-phosphorus detector) GC-MS mit PCI (=positive chem. ionization)
Result: concentrations in water samples:
Station A: von < 1 ng/l bis 0.9 ug/l
Station B: < 1 ng/l (= not detected)
Source: BASF AG Ludwigshafen

(24)

Type of measurement: other
Medium: surface water

Remark: sampling area: Nilwala River in Southern Sri Lanka
sampling time: april 1988
sample preparation: extraction with petrol ether /dichloro-methane
analytical method: GC with PND (= nitrogen-phoshorous detektor)
Result: concentration: about 10 ng/l
Source: BASF AG Ludwigshafen

(25)

Type of measurement: other
Medium: surface water

Remark: sampling area: Llobregat, Besos River in Spain
sampling time: march 1985 to march 1986
sampling preparation: CLST (=closed loop stripping technique)
analytical methods: GC-FID; GC-MS
Result: concentrations: Llobregat: 20-2000 ng/l
Besos: 10-24000 ng/l
Source: BASF AG Ludwigshafen

(26)

Type of measurement: other
Medium: surface water

Remark: sampling area: la Pineda beach; Vilanova-Sitges coast; Spain
sampling time: february 1986
sample preparation: CLST (= closed loop stripping technique)
analytical methods: GC-FID bzw. GC-MS
Result: concentrations: No tributylphospates have been detected.
Source: BASF AG Ludwigshafen

(27)

Type of measurement: other
Medium: surface water

Remark: sampling area: River Po (Station A); Adriatic Sea: Lido delle Nazioni (Station B) und Marina di Ravenna (Station C); Italy
sampling time: april to august 1988
sample preparation: extraction with dichloromethane
analytical method: GC, silica columns (SP 255, OV 1701), carrier gas: helium; NPD-detector
Result: concentrations: Station A: 219,17,192,29 ng/l
Station B: 53,71,228 ng/l
Station C: 33,84,33 ng/l

Source: BASF AG Ludwigshafen

(28)

Type of measurement: other
Medium: surface water

Remark: sampling area: River Po, River Lambra, Italy
sampling time: march 1985 (sept. 1985)
sample preparation: extraction with XAD2,XAD7-resins,acetone
analytical method: GC-FID
Result: concentrations: River Lambra: 0,01; 0,4 (0,5) ug/l
River Po: 0,06(0,04); 0,14(0,2), 0,2 ug/l
Source: BASF AG Ludwigshafen

(29)

Type of measurement: other
Medium: other

Remark: sampling area: Northern Italy
samling time: feb./april 1987
analytical method: GC-NPD
Result: conc.: River Po (Turin, Ferrara): 0,033-0,136 ng/l
River Adige (Cavanella): 0,014; 0,017 ng/l
Lake Como (Como): 0,57 ng/l
ground water (Dalamine): 0,001 ng/l
Source: BASF AG Ludwigshafen

(30)

Type of measurement: other
Medium: sediment

Remark: sampling area: Lake Varese, Lake Comabbio, Lake Monate (Northern Italy)
sampling time: may 1986; sept.1987
analytical method: GC-NPD
Result: Triisobutylphosphate has been detected in sediment extracts, but also in the analytical blank at levels comparable to those of the samples.
Source: BASF AG Ludwigshafen

(31)

Type of measurement: other
Medium: surface water

Remark: sampling area: Llobregat, Ter Rivers (Spain)
sampling time: sept. 1989 - march 1990
sample preparation: CLSA-Extrakte

analytical method: GC-FID; GC-MS
Result: concentrations: Llobregat River: 2,2-15 ug/l
Llobregat (tap water): 3,1-18 ug/l
Ter River (tap water): n.d.
Conc.= sum of tri-iso- and tri-n-butyl phosphate.
Source: BASF AG Ludwigshafen

(32)

Type of measurement: other
Medium: surface water

Remark: sampling area: Llobregat, Ter Rivers (Spain)
sampling time: weekly about 9 months
sample preparation: CLSA
analytical methods: GC-FID; GC-MS
Result: concentrations: Llobregat(raw): 0,6-21,5 ug/l
Llobregat(tap water): 0,26-18 ug/l
Ter(drinking water): nd-0,6 ug/l
Source: BASF AG Ludwigshafen

(33)

Type of measurement: other
Medium: surface water

Remark: sampling area: River Waal bei Brakel, Netherlands
sampling time: april 1974
sample preparation: Extraction with hexane
analytical methods: GC-MS
Result: Triisobutylphosphate has been detected qualitative.
Source: BASF AG Ludwigshafen

(34)

Type of measurement: other
Medium: surface water

Remark: Untersuchungsgebiet: Aestuarien von Elbe, Weser u. Ems; Deutschland
Untersuchungszeitraum: 1977-1983
Probenvorbereitung: Extraktion mit Hexan
Analysenmethode: GC-ECD bzw. GC-FID; GC-MS
Result: Tributylphosphate wurden in Elbe und Weser in Konzentrationsbereichen von 20 bis 100 ng/l und in der Ems von 100 bis 500 ng/l nachgewiesen. (halbquantitativ)
Source: BASF AG Ludwigshafen

(35)

Type of measurement: other

Medium: other

Remark: sampling area: Barcelona, Besos River (Spain)
sampling time: march-july 1987
analytical method: HRGC-NPD

Result: Triisobutylphosphate was identified in wastewaters, seawater and sediments.

Source: BASF AG Ludwigshafen

(36)

Type of measurement: other
Medium: other: Abwasser

Remark: Untersuchungsort: Unterweser im bremischen Raum (Klaeranlagen Seehausen, Delmenhorst, Osterholz, Farge, Bremerhaven, Bremer Wollkaemmerei, Kloeckner Werke)
Analysenmethode: Extraktion mit n-Hexan/Dichlormethan, GC-PND mit 2 Kapillarsaeulen

Result: mittlere Konzentration im Abwasser: ca. 500 ng/l
Einzelwerte (in ng/l): Klaeranlagen Seehausen: 551-8070; Delmenhorst: 110-13600; Osterholz: 310-2610; Farge: 680-3000; Bremer Wollkaemmerei: 761-4400; Kloeckner Werke: 450-1340

Source: BASF AG Ludwigshafen

(37)

Type of measurement: other
Medium: surface water

Remark: sampling area: Llobregat River (Station A); Ebro River mouth (Station B) in Spain
sampling time: march to june 1988
sample preparation: extraction with methylene chloride
Analytical method: GC-NPD (= nitrogen-phosphorus detector)
GC-MS mit PCI (=positive chem. ionization)

Result: concentrations in water samples:
Station A: von < 1 ng/l bis 0.9 ug/l
Station B: < 1 ng/l (= not detected)

Source: BASF AG Ludwigshafen

(38)

Type of measurement: other
Medium: surface water

Remark: sampling area: Nilwala River in Southern Sri Lanka
sampling time: april 1988
sample preparation: extraction with petrol ether

/dichloro-methane
analytical method: GC with PND (= nitrogen-phoshorous detektor)
Result: concentration: about 10 ng/l
Source: BASF AG Ludwigshafen

(39)

Type of measurement: other
Medium: surface water

Remark: sampling area: Llobregat, Besos River in Spain
sampling time: march 1985 to march 1986
sampling preparation: CLST (=closed loop stripping technique)
analytical methods: GC-FID; GC-MS
Result: concentrations: Llobregat: 20-2000 ng/l
Besos: 10-24000 ng/l
Source: BASF AG Ludwigshafen

(40)

Type of measurement: other
Medium: surface water

Remark: sampling area: la Pineda beach; Vilanova-Sitges coast; Spain
sampling time: february 1986
sample preparation: CLST (= closed loop stripping technique)
analytical methods: GC-FID bzw. GC-MS
Result: concentrations: No tributylphospates have been detected.
Source: BASF AG Ludwigshafen

(41)

Type of measurement: other
Medium: surface water

Remark: sampling area: River Po (Station A); Adriatic Sea: Lido delle Nazioni (Station B) und Marina di Ravenna (Station C); Italy
sampling time: april to august 1988
sample preparation: extraction with dichloromethane
analytical method: GC, silica columns (SP 255, OV 1701), carrier gas: helium; NPD-detector
Result: concentrations: Station A: 219,17,192,29 ng/l
Station B: 53,71,228 ng/l
Station C: 33,84,33 ng/l
Source: BASF AG Ludwigshafen

(42)

Type of measurement: other
Medium: surface water

Remark: sampling area: River Po, River Lambra, Italy
sampling time: march 1985 (sept. 1985)
sample preparation: extraction with XAD2,XAD7-resins,acetone
analytical method: GC-FID
Result: concentrations: River Lambra: 0,01; 0,4 (0,5) ug/l
River Po: 0,06(0,04); 0,14(0,2), 0,2 ug/l
Source: BASF AG Ludwigshafen

(43)

Type of measurement: other
Medium: other

Remark: sampling area: Northern Italy
samling time: feb./april 1987
analytical method: GC-NPD
Result: conc.: River Po (Turin, Ferrara): 0,033-0,136 ng/l
River Adige (Cavanella): 0,014; 0,017 ng/l
Lake Como (Como): 0,57 ng/l
ground water (Dalamine): 0,001 ng/l
Source: BASF AG Ludwigshafen

(44)

Type of measurement: other
Medium: sediment

Remark: sampling area: Lake Varese, Lake Comabbio, Lake Monate
(Northern Italy)
sampling time: may 1986; sept.1987
analytical method: GC-NPD
Result: Triisobutylphosphate has been detected in sediment extracts, but also in the analytical blank at levels comparable to those of the samples.
Source: BASF AG Ludwigshafen

(45)

Type of measurement: other
Medium: surface water

Remark: sampling area: Llobregat, Ter Rivers (Spain)
sampling time: sept. 1989 - march 1990
sample preparation: CLSA-Extrakte
analytical method: GC-FID; GC-MS
Result: concentrations: Llobregat River: 2,2-15 ug/l
Llobregat (tap water): 3,1-18 ug/l
Ter River (tap water): n.d.
Conc.= sum of tri-iso- and tri-n-butyl phosphate.

Source: BASF AG Ludwigshafen

(46)

Type of measurement: other
Medium: surface water

Remark: sampling area: Llobregat, Ter Rivers (Spain)
sampling time: weekly about 9 months
sample preparation: CLSA
analytical methods: GC-FID; GC-MS
Result: concentrations: Llobregat(raw): 0,6-21,5 ug/l
Llobregat(tap water): 0,26-18 ug/l
Ter(drinking water): nd-0,6 ug/l
Source: BASF AG Ludwigshafen

(47)

Type of measurement: other
Medium: surface water

Remark: sampling area: River Waal bei Brakel, Netherlands
sampling time: april 1974
sample preparation: Extraction with hexane
analytical methods: GC-MS
Result: Triisobutylphosphate has been detected qualitative.
Source: BASF AG Ludwigshafen

(48)

Type of measurement: other
Medium: surface water

Remark: Untersuchungsgebiet: Aestuarien von Elbe, Weser u. Ems; Deutschland
Untersuchungszeitraum: 1977-1983
Probenvorbereitung: Extraktion mit Hexan
Analysenmethode: GC-ECD bzw. GC-FID; GC-MS
Result: Tributylphosphate wurden in Elbe und Weser in Konzentrationsbereichen von 20 bis 100 ng/l und in der Ems von 100 bis 500 ng/l nachgewiesen. (halbquantitativ)
Source: BASF AG Ludwigshafen

(49)

Type of measurement: other
Medium: other

Remark: sampling area: Barcelona, Besos River (Spain)
sampling time: march-july 1987

analytical method: HRGC-NPD
Result: Triisobutylphosphate was identified in wastewaters, seawater and sediments.
Source: BASF AG Ludwigshafen

(50)

3.2.2 Field Studies

-

3.3.1 Transport between Environmental Compartments

Type: adsorption
Method: other: berechnet (PCKOC, Howard/Meylan, 1993)

Remark: Adsorption im Boden: Koc = 1112
Source: BASF AG Ludwigshafen

(15)

Type: adsorption
Method: other: berechnet (PCKOC, Howard/Meylan, 1993)

Remark: Adsorption im Boden: Koc = 1112
Source: BASF AG Ludwigshafen

(16)

3.3.2 Distribution

Method: Calculation according Mackay, Level I
Year: 1995

Remark: Bevorzugte Zielkompartimente:

Luft (16%), Wasser (46%), Boden (16%), Sediment (18%).
Wegen ungenauer Dampfdruckangabe kann das Ergebnis nicht als valide angesehen werden.
Zugrundeliegende Daten fuer die Berechnung:
Wasserloeslichkeit 265 mg/l
Dampfdruck 1 Pa (umgerechnet)
log Pow 3.72
Source: BASF AG Ludwigshafen

(51) (52)

Method: Calculation according Mackay, Level I
Year: 1995

Remark: Bevorzugte Zielkompartimente:
Luft (16%), Wasser (46%), Boden (16%), Sediment (18%).
Wegen ungenauer Dampfdruckangabe kann das Ergebnis nicht als valide angesehen werden.
Zugrundeliegende Daten fuer die Berechnung:
Wasserloeslichkeit 265 mg/l
Dampfdruck 1 Pa (umgerechnet)
log Pow 3.72
Source: BASF AG Ludwigshafen

(51) (53)

3.4 Mode of Degradation in Actual Use

Remark: no data are available
Source: BASF AG Ludwigshafen

3.5 Biodegradation

Type: aerobic
Inoculum: other: BASF-Belebtschlamm
Degradation: = 97 % after 14 day(s)
Result: other: DOC-Abnahme
Kinetic:

3 hour(s)	= 5 %
2 day(s)	ca. 20 %
5 day(s)	ca. 94 %

Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1990
GLP: no
Test substance: other TS: geprueft als Etingal (= Triisobutylphosphat)

Source: BASF AG Ludwigshafen

(54)

Type: aerobic
Inoculum: other: BASF-Belebtschlamm
Degradation: = 97 % after 14 day(s)
Result: other: DOC-Abnahme
Kinetic:
3 hour(s) = 5 %
2 day(s) ca. 20 %
5 day(s) ca. 94 %

Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1990
GLP: no
Test substance: other TS: geprueft als Etingal (= Triisobutylphosphat)

Source: BASF AG Ludwigshafen

(55)

Type: aerobic
Inoculum: other bacteria: Klaeranlagenablauf, kommunal
Degradation: = 70 % after 35 day(s)
Result: other: DOC-Abnahme
Kinetic:
3 day(s) ca. 5 %
5 day(s) ca. 13 %
21 day(s) ca. 59 %
27 day(s) ca. 63 %

Method: other: Modifizierter OECD-Screening-Test (Amtsblatt d.Europ.Gemein- schaften, L 251, 1984, C 3);
Year: 1990
GLP: no
Test substance: other TS: geprueft als Etingal (=Triisobutylphosphat)

Source: BASF AG Ludwigshafen

(56)

Type: aerobic
Inoculum: other bacteria: Klaeranlagenablauf, kommunal
Degradation: = 70 % after 35 day(s)
Result: other: DOC-Abnahme
Kinetic:
3 day(s) ca. 5 %
5 day(s) ca. 13 %
21 day(s) ca. 59 %
27 day(s) ca. 63 %

Method: other: Modifizierter OECD-Screening-Test (Amtsblatt d.Europ.Gemeinschaften, L 251, 1984, C 3)
Year: 1990
GLP: no
Test substance: other TS: geprueft als Etingal (=Triisobutylphosphat)

Source: BASF AG Ludwigshafen

(57)

Type: aerobic
Inoculum: other: BASF-Belebtschlamm
Result: other: schwer biologisch abbaubar

Method: other: Sapromat-Test (BASF-Methode)
Year: 1984
GLP: no

Remark: O2/C-Verhältnis
Source: BASF AG Ludwigshafen

(58)

3.6 BOD5, COD or BOD5/COD Ratio

Method: other: DIN 38409/51
Year: 1984
GLP: no

C O D

Method: other: DIN 38409/41
Year: 1984
GLP: no
COD: = 944 mg/g substance

R A T I O B O D 5 / C O D

BOD5/COD: < .002
Method:
Remark: BOD5 < 2 mg/g
Source: BASF AG Ludwigshafen

(59)

Method: other: DIN 38409/51
Year: 1984
GLP: no

C O D

Method: other: DIN 38409/41
Year: 1984
GLP: no
COD: = 944 mg/g substance

R A T I O B O D 5 / C O D

BOD5/COD: < .002
Method:
Remark: BOD5 < 2 mg/g
Source: BASF AG Ludwigshafen

(60)

3.7 Bioaccumulation

Remark: no data are available
Source: BASF AG Ludwigshafen

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
NOEC: 9.4
LC50: 23

Method: other: according to U.S. EPA
GLP: yes
Test substance: other TS

Source: BASF AG Ludwigshafen
Test substance: Tris(2-Methylpropyl)ester CAS:(126-71-6)

(61)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no

Method: other
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Fingerlinge; 2 Fische eingesetzt; einzige getestete Konzentration: 5 mg/l; keine Effekte beobachtet.
Source: BASF AG Ludwigshafen

(62)

Type: static
Species: Leuciscus idus (Fish, fresh water)

Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 17.8 - 21.5

Method: other: in Anlehnung an: "Akuter Fischtest", Entwurf der GDCh-Arbeitsgruppe, Stand 16.09.77 (zukuenftig DIN 38412, Teil 15,"Goldorfentest")
Year: 1979
GLP: no
Test substance: other TS

Source: BASF AG Ludwigshafen
Test substance: Es wurde Etingal A geprueft, das neben Triisobutylphosphat noch ca. 10% Isobutanol enthaelt.

(63)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no

Method: other
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Fingerlinge; 2 Fische eingesetzt; einzige getestete Konzentration: 5 mg/l; keine Effekte beobachtet.
Source: BASF AG Ludwigshafen

(62)

Type: static
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: = 20

Method: other: in Anlehnung an: Japanese Industrial Standard, K 0102, 1974
GLP: no
Test substance: other TS

Source: BASF AG Ludwigshafen
Test substance: Es wurde Etingal A geprueft, das neben Triisobutylphosphat noch ca. 10 % Isobutanol enthaelt.

(64)

Type: static
Species: Petromyzon marinus
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no

Method: other
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Larven; 2 Tiere eingesetzt; einzige getestete Konzentration: 5 mg/l; keine Effekte beobachtet.
Source: BASF AG Ludwigshafen

(62)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC0: = 10
EC50: = 16
EC100: = 58

Method: other: Daphnien-Kurzzeittest nach DIN 38412/11
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.10 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: Isobutanol < 0,5 %, Monoisobutylphosphat, Diisobutylphosphat

(65)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring:
EC0: = 10

EC50: = 16
EC100: = 58

Method: other: Daphnien-Kurzzeittest nach DIN 38412/11
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.10 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: Isobutanol < 0,5 %, Monoisobutylphosphat, Diisobutylphosphat

(66)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
EC0: = 5.8
EC50: = 11
EC100: = 18

Method: other: Daphnien-Kurzzeittest nach DIN 38412/11
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.10 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: Isobutanol < 0,5 %, Monoisobutylphosphat, Diisobutylphosphat

(65)

Species: Daphnia magna (Crustacea)

Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
EC0: = 5.8
EC50: = 11
EC100: = 18

Method: other: Daphnien-Kurzzeittest nach DIN 38412/11
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.10 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: Isobutanol < 0,5 %, Monoisobutylphosphat, Diisobutylphosphat

(66)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring:
EC10: = 24
EC50: = 33

Method: other: Algen-Zellvermehrungs-Hemmtest nach DIN 38412/9
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.5 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0,5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(65)

Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring:
EC10: = 24
EC50: = 33

Method: other: Algen-Zellvermehrungs-Hemmtest nach DIN 38412/9
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.5 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0,5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(66)

Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
EC10: = 22
EC50: = 30

Method: other: Algen-Zellvermehrungshemmtest nach DIN 38412/9
Year: 1989

GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.5 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0,5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(65)

Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
EC10: = 22
EC50: = 30

Method: other: Algen-Zellvermehrungshemmtest nach DIN 38412/9
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.5 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0,5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(66)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring:
EC10: = 25
EC50: = 34

Method: other: Algen-Zellvermehrungshemmtest nach DIN 38412/9
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.5 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0.5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(65)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring:

EC10: = 25
EC50: = 34

Method: other: Algen-Zellvermehrungshemmtest nach DIN 38412/9
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.5 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0.5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(66)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
EC10: = 13
EC50: = 18

Method: other: Algen-Zellvermehrungshemmtest nach DIN 38412/9
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.5 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0.5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(65)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
EC10: = 13
EC50: = 18

Method: other: Algen-Zellvermehrungshemmtest nach DIN 38412/9
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.5 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0.5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(66)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 30 minute(s)
Unit: mg/l Analytical monitoring:
EC10: = 280
EC50: = 440
EC90 : = 880
TGK : = 280

Method: other: Pseudomonas-Atmungs-Hemmtest nach DIN 38412/27
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.100 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0.5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(65)

Type: aquatic
Species: Pseudomonas putida (Bacteria)

Exposure period: 30 minute(s)
Unit: mg/l Analytical monitoring:
EC10: = 280
EC50: = 440
EC90 : = 880
TGK : = 280

Method: other: Pseudomonas-Atmungs-Hemmtest nach DIN 38412/27
Year: 1989
GLP: no
Test substance: other TS

Remark: Loesungsvermittler: Cremophor (max.100 mg/l)
Source: BASF AG Ludwigshafen
Test substance: ca. 98 % Triisobutylphosphat, Verunreinigungen: < 0.5 % Isobutanol, Monoisobutylphosphat, Diisobutylphosphat

(66)

Type: aquatic
Species: other bacteria: BASF-Belebtschlamm
Exposure period: 30 minute(s)
Unit: mg/l Analytical monitoring:
EC20 : = 390

Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
GLP: no

Source: BASF AG Ludwigshafen

(59)

Type: aquatic
Species: other bacteria: BASF-Belebtschlamm
Exposure period: 30 minute(s)
Unit: mg/l Analytical monitoring:
EC20 : = 390

Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
GLP: no

Source: BASF AG Ludwigshafen

(60)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Remark: no data are available
Source: BASF AG Ludwigshafen

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Sediment Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants

Remark: no data are available
Source: BASF AG Ludwigshafen

4.6.3 Toxicity to Soil Dwelling Organisms

Remark: no data are available
Source: BASF AG Ludwigshafen

4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

Remark: no data are available
Source: BASF AG Ludwigshafen

4.7 Biological Effects Monitoring

Remark: no data are available
Source: BASF AG Ludwigshafen

4.8 Biotransformation and Kinetics

Remark: no data are available
Source: BASF AG Ludwigshafen

4.9 Additional Remarks
-

5.0 Toxicokinetics, Metabolism and Distribution
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Value: = 4180 mg/kg bw

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(67)

Type: LD50
Species: rat
Value: 3072 - 6144 mg/kg bw

Method: other

GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(68)

Type: LD50
Species: rat
Value: > 5000 mg/kg bw

Method: other: nach FIFRA-Guideline bzw. TSCA-Guideline
Year: 1982
GLP: yes

Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(69)

Type: LD50
Species: rat
Value: 6400 - 12800 mg/kg bw

Method: other: no data
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(70)

Type: LD50
Species: mouse
Value: 3200 - 6400 mg/kg bw

Method: other: no data
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(70)

Type: LD50
Species: hen
Value: 1500 mg/kg bw

Method: other
GLP: no data
Test substance: other TS

Source: BASF AG Ludwigshafen
Test substance: Tributylphosphat, ohne weitere Angaben ob n-Butyl-, Isobutyl- oder tert. Butylphosphat bzw. Gemisch.

(71)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Exposure time: 4 hour(s)
Value: > 5.14 mg/l

Method: OECD Guide-line 403 "Acute Inhalation Toxicity"

Year: 1981
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(72)

Type: other
Species: rat
Exposure time: 6 hour(s)

Method: other: no data
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Keine Mortalitaet nach 6 Stunden Exposition gegenueber einerTestsubstanzkonzentration von 50 ppm (0.55 mg/l); vollstaendige Mortalitaet nach 6 Stunden Exposition gegenueber einer Testsubstanzkonzentration von 7500 ppm (82.8 mg/l) innerhalb von 48 Stunden.
Source: BASF AG Ludwigshafen

(70)

Type: other: IRT
Species: rat
Exposure time: 6 hour(s)
Value: 1.35 mg/l

Method: other
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: 0/3, Reizwirkung, keine Laehmungen, zentrale Erregung
Source: BASF AG Ludwigshafen

(68)

Type: other: Aerosolversuch
Species: mammal
Exposure time: 30 minute(s)
Value: 52 mg/l

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Wert: (Nominalkonzentration): Katze Speichelfluss, Reizwirkung auf Schleimhaut und Atemwege; Kaninchen keine Angaben; Ratte und Maus Dyspnoe, Todesfaelle.
Source: BASF AG Ludwigshafen

(67)

Type: other: IRT
Species: mammal
Exposure time: 6 hour(s)
Value: 1.7 mg/l

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Wert: Nominalkonz.
Katze Speichelfluss; Maus Todesfaelle; andere o.b.B.
Source: BASF AG Ludwigshafen

(73)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Value: > 5000 mg/kg bw

Method: other: nach FIFRA-Guideline bzw. TSCA-Guideline
Year: 1982
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(74)

Type: LD50
Species: guinea pig
Value: > 9600 mg/kg bw

Method: other: no data
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Originalangabe: LD50 > 10000 ul/kg

Source: BASF AG Ludwigshafen

(70)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: rat
Route of admin.: i.p.
Value: 768 - 1536 mg/kg bw

Method: other
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(68)

Type: LD50
Species: rat
Route of admin.: i.p.
Value: 200 - 400 mg/kg bw

Method: other: no data
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(70)

Type: LD50
Species: mouse
Route of admin.: i.p.
Value: 800 - 1600 mg/kg bw

Method: other: no data
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(70)

Type: LD50
Species: mouse
Route of admin.: s.c.
Value: = 2850 mg/kg bw

Method: other: BASF-Test

GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(67)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Result: irritating

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(75)

Species: rabbit
Result: not irritating
EC classificat.: not irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1981
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(76)

Species: rabbit
Result: slightly irritating

Method: other: nach FIFRA-Guideline bzw. TSCA-Guideline (intakte Haut, 4h, semi-okklusiv)
Year: 1982
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(77)

Species: guinea pig

Method: other: no data
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Ergebnis nicht eindeutig; laut Angabe der Autoren schwaecher reizend als das stark reizende Tributylphosphat (keine weiteren Angaben).
Source: BASF AG Ludwigshafen

(70)

5.2.2 Eye Irritation

Species: rabbit
Result: irritating

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(75)

Species: rabbit
Result: not irritating
EC classificat.: not irritating

Method: other: nach FIFRA-Guideline bzw. TSCA-Guideline
Year: 1982
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: Nach Guideline nicht reizend.
Source: BASF AG Ludwigshafen

(78)

5.3 Sensitization

Type: Buehler Test
Species: guinea pig
Result: sensitizing
Classification: sensitizing

Method: OECD Guide-line 406 "Skin Sensitization"
Year: 1992
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen
Test substance: Etingal, Bach MG 94-37
Carrier Olive oil DAB 10

(79)

Type: Guinea pig maximization test
Species: guinea pig
Result: sensitizing
Classification: sensitizing

Method: OECD Guide-line 406 "Skin Sensitization"
Year: 1981
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Source: BASF AG Ludwigshafen

(80)

Type: no data
Species: guinea pig
Result: sensitizing

Method: other: no data
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Laut Angabe der Autoren ist von einer sensibilisierenden Wirkung auszugehen, obwohl dies nicht eindeutig gezeigt werden konnte.
Source: BASF AG Ludwigshafen

(70)

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of administration: oral feed
Exposure period: 13 Wochen
Frequency of treatment: kontinuierlich im Futter
Post exposure period: keine bzw. 8 Wochen
Doses: 13.9-16.8, 68.4-84.3, 346.1-403.9 mg/kg/d (200, 1000, 5000 ppm im Futter)
Control Group: yes, concurrent no treatment
NOAEL: 68.4 - 84.3 mg/kg bw

Method: other
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Remark: In der Kontrollgruppe und der hoechsten Dosisgruppe wurden jeweils 30 maennliche und 30 weibliche, in der niedrigen undder mittleren Dosisgruppe jeweils 10 maennliche und 10 weibliche Tiere eingesetzt. Die Tiere der Kontroll- und der hoechsten Dosisgruppe wurden 8 Wochen nachbeobachtet. Untersucht wurde der Zustand der Tiere, das Koerpergewicht, die Organgewichte (Leber, Nieren, Nebennieren, Testes), haematologische und Serumparameter, Histologie der unterschiedlichsten Gewebe (Kontroll- und hoechste Dosisgruppe).
Result: Es wurde keine Mortalitaet festgestellt. In der hoechsten Dosisgruppe wurde verminderte Futteraufnahme festgestellt; haematologisch zeigte sich eine leicht verminderte Zahl von Neutrophilen; die Cholesterol-Werte waren erhoeht. Weitere substanzbedingte Veraenderungen wurden im Vergleich zur Kontrolle nicht festgestellt.

Remark: In the control group and in the highest dose group, 30 male and 30 female animals were used; in the lowest and in the middle dose group, 10 male and 10 female animals were used. The animals in the control group and in the highest dose group were observed for eight weeks.

The condition of the animals was examined, body weight, organ weights (liver, kidneys, suprarenal bodies, testes), hematological and blood serum parameters, histology and the most different tissues (control and highest dose group).

Result: No mortalities were found. In the highest dose group, a reduced feed intake was found; hematological parameters showed a slight reduction in the number of neutrophiles; the cholesterol value was elevated. No further substance-dependent changes in comparison to the control were found.

Source: BASF AG Ludwigshafen

(81) (82)

Species: rat Sex: male/female
Strain: no data
Route of administration: other: Pfefferminztee (in der Traenke)
Exposure period: 51 Tage
Frequency of treatment: taeglich
Post exposure period: keine Angabe
Doses: 6316 ppm (entspr. 430-440 mg/kg/Tag; m-w)
Control Group: yes, concurrent vehicle

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Result: Kein Einfluss auf die Koerpergewichtsentwicklung, vermehrtes Auftreten von "Nierenreizungen" im Vergleich zur Kontrollgruppe (wird von den Autoren als belanglos bezeichnet).
Source: BASF AG Ludwigshafen

(83)

Species: rabbit Sex: male/female
Strain: no data
Route of administration: gavage
Exposure period: a) 3 x in 5 Tagen b) 22 x in 30 Tagen
Frequency of treatment: keine Angabe
Post exposure period: keine Angabe
Doses: a) 960 mg/kg b) 480 mg/kg
Control Group: no data specified

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Durch die geringe Tierzahl und teilweise Spontanerkrankung der Tiere, ist diese alte Studie nicht voll valide.
Result: Pro Dosis wurde nur je 1 Tier eingesetzt, beide Tiere sind gestorben
a) Diarrhoe, nekrotische Veraenderungen der Darmschleimhaut
b) Gewichtsverlust, Granulozytose und Lymphopenie,

Protein- und Glucosurie, eitrige Pneumonie und haemorrhagische Enteritis.
Source: BASF AG Ludwigshafen

(83)

Species: cat Sex: no data
Strain: no data
Route of administration: gavage
Exposure period: siehe Text
Frequency of treatment: 3 x bis 38 x
Post exposure period: Nachbeobachtungszeit bis 51 Tage
Doses: 950; 475; 95; 47,8 mg/kg siehe auch Text
Control Group: no data specified

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Durch die geringe Tierzahl und teilweise Spontanerkrankung der Tiere, ist diese alte Studie nicht voll valide.
Result: 960 mg/kg (5x; 5 Tage): Todesfall, Speichelfluss, Gleichgewichtsstoe- rungen, Durchfall, Kraempfe, Leukozytose mit Granulozytose und Lymphopenie, Proteinurie.
480 mg/kg (3x; 7 Tage): Todesfall (starke Leukopenie haemorrhagische Diathese) Speichelfluss, Erregung, Gleichgewichtsstoerungen, Harnveraenderungen, Erholung in der Nachbeobachtungszeit. 96 mg/kg (25x; 35 Tage und 38x; 52 Tage): Todesfall (eitrige Bronchopneumonie), Inappetenz, Durchfall, Somnolenz, Erholung in der Nachbeob- achtungszeit.
48 mg/kg (23x; 39 Tage): Sporadischer Durchfall, sonst keine klinischen, haematologischen oder Harnveraenderungen.
Source: BASF AG Ludwigshafen

(83)

Species: mammal Sex: no data
Strain: no data
Route of administration: inhalation
Exposure period: 4 Tage

Frequency of treatment: 6 h/Tag
Post exposure period: keine Angabe
Doses: gesaettigte Atmosphaere (Zimmertemperatur) entspr. 0,3-1 mg/l
Control Group: no data specified

Method: other: BASF-Test
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Durch die geringe Tierzahl und teilweise Spontanerkrankung der Tiere, ist diese alte Studie nicht voll valide.
Result: 1 Maus unter Dyspnoe gestorben, sonst symptomlos vertragen.
Source: BASF AG Ludwigshafen

(83)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium; TA98 TA100 TA1535 TA1537
Concentration: 20 ug - 5000 ug/plate (SPT); 15 ug - 5000 ug/plate (PIT)
Metabolic activation: with and without
Result: negative

Method: OECD Guide-line 471
Year: 1983
GLP: no
Test substance: as prescribed by 1.1 - 1.4

Remark: Standard plate (SPT) und preincubation test (PIT)
Source: BASF AG Ludwigshafen

(84)

Type: Ames test
System of testing: Salmonella typhimurium TA1535, TA1537, TA1538, TA98, TA100
Concentration: 10 - 5000 ug/plate
Metabolic activation: with and without
Result: negative

Method: OECD Guide-line 471
Year: 1983
GLP: yes

Test substance: as prescribed by 1.1 - 1.4

Remark: Plate incorporation test; pre-incubation test
Source: BASF AG Ludwigshafen

(85)

Type: Ames test
System of testing: Salmonella typhimurium TA98, TA1535, TA1537, TA100
Concentration: up to 5 mg/plate
Metabolic activation: with and without
Result: negative

Method: other: according to Ames 1975
GLP: no data
Test substance: other TS

Remark: plate incorporation test
Source: BASF AG Ludwigshafen
Test substance: CAS 126-71-6 : purity 99.78%, solution anhydrous aceton

(86)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse Sex: male/female
Strain: CD-1
Route of admin.: i.p.
Doses: 300, 600 and 1200 mg/kg

Method: other: according the EPA Gene-Tox program
GLP: yes
Test substance: other TS

Remark: positive control: Cyclophosphamide 60 mg/kg bw, sampling time 24h
test article: sampling time 24, 48, 72 hours
5 animals/sex/time were scored for the occurence of micronucleated PCE and PCE/erythrocyte ratios.
Result: The highest dose level 1200 mg/kg bw did not induce statistically significant decreases in mean PCE/erythrocyte ratios or increases in frequency of micronucleated PCEs.
Result: negative
Source: BASF AG Ludwigshafen
Test substance: substance CAS: 126-71-6

vehicle: corn oil (10 ml of solution(/kg bw)

(87)

5.7 Carcinogenicity
-

5.8.1 Toxicity to Fertility
-

5.8.2 Developmental Toxicity/Teratogenicity

Species:	rat	Sex: female
Strain:	other: CD (SD) BR VAF/Plus strain	
Route of administration:	gavage	
Exposure period:	6. bis 15. Tag der Gestation	
Frequency of treatment:	taeglich	
Duration of test:	21 Tage	
Doses:	100; 300; 1000 mg/kg in 0.5 % Natrium Carboxylmethylcellulose	
Control Group:	yes, concurrent no treatment	

Method:	OECD Guide-line 414 "Teratogenicity"
Year:	1981
GLP:	yes
Test substance:	as prescribed by 1.1 - 1.4

Remark: Nachbeobachtung: bis zum 20. Tag der Gestation

Result: Pro Versuchsgruppe wurden je 25 Muttertiere eingesetzt. Ein dosisabhaengiger Speichelfluss wurde in allen Versuchsgruppen beobachtet. Im Anschluss an die Applikation dauerte dieser Speichelfluss in der hoechsten Dosierungsgruppe etwa 3 Stunden an, in den anderen Gruppen war er maximal eine Stunde zu beobachten. Die Anzahl der betroffenen Tiere in der 100 mg/kg Gruppe war geringer.
In der 1000 mg/kg Gruppe war der Trinkwasserverbrauch waehrend der Applikationsdauer erhoeht, in der Nachbeobachtungsphase sank er aber wieder auf den Kontrollwert ab. In allen Gruppen wurde keine Aenderung der Futteraufnahme beobachtet. Die Koerpergewichtszunahme in der hoechsten Dosisgruppe war ab Tag 8 der Gestation leicht verringert, erreichte aber zum Ende der Studie wieder den Kontrollwert. In den anderen Versuchsgruppen wurde kein Unterschied zur Kontrolle beobachtet.
In der 1000 mg/kg Gruppe war die Inzidenz des fruehen Embryonal-Tods leicht erhoeht. Dieser Befund war aber statistisch nicht signifikant. Da keine weiteren Effekte beobachtet wurden, wurde dieser Befund als zweifelhaft eingestuft.
Eine substanzbedingte Beeinflussung der Zahl der Fehlbildungen und Variationen wurde nicht beobachtet.

Remark: Post-observation: Until day 20 of gestation

Result: Approximately 25 mother animals were used for the test groups. A dose-dependent flow of saliva was observed in all test groups. In connection with the application, the flow of saliva continued for about 3 hours in the highest dose group; in the other groups, a maximum duration of one hour was observed. The number of affected animals in the 100-mg/kg group was smaller.

The consumption of drinking water was heightened during the application time in the 1000-mg/kg group, in the observation phase it dropped back again to the control value. There were no changes observed in the feed uptake in any groups. The increase in body weight in the highest dose group was slightly reduced after the 8th day of gestation, but it reached the control value again by the end of the study. In the other test groups, no differences from the control were observed.

The incidence of early embryonic mortality was slightly higher in the 1000-mg/kg group; however, this finding was not statistically significant. Because there were no other effects observed, this finding was classified as dubious.

No substance-dependent influence on the number of mutations and variations was observed.

Source: BASF AG Ludwigshafen

(88)

5.8.3 Toxicity to Reproduction, Other Studies

-

5.9 Specific Investigations

-

5.10 Exposure Experience

Remark:	Es liegen keine Untersuchungsberichte ueber Erfahrungen beim Menschen vor.
Source:	BASF AG Ludwigshafen

5.11 Additional Remarks

Type: Neurotoxicity

Remark: Akute verzoegerte Neurotoxizitaet beim Huhn:
Sondierung, 500 und 1000 mg/kg 1x, 42 d Nachbeobachtung
2000 und 5000 mg/kg 2x im Abstand von 21 d, 42 d
Nachbeobachtung Vehikelkontrolle Olivenoel, Positivkontrolle
Triorthokresylphosphat.
Substanz in allen Dosisgruppen: Keine klinischen
Beeintraechtigungen insbesondere keine neurotoxischen
Symptome. Positivkontrolle 7/15 neurotoxische Symptome,
5/15 gestorben.
Source: BASF AG Ludwigshafen
Test substance: Triisobutylphosphat

(89)

Type: Neurotoxicity

Remark: Es wurde die Auswirkung einer oralen Einzeldosis der
Testsubstanz auf verschiedene Enzymaktivitaeten (neurotox.
Esterase und Acetylcholinesterase im Gehirn,
Butyrylcholinesterase im Plasma) beim Huhn untersucht. In
einer vorab durchgefuehrten "range-finding" Studie wurde
den Tieren die Testsubstanz in einem Dosisbereich zwischen
1000 und 5000 mg/kg verabreicht. In den beiden hoechsten
Dosisgruppen von 4000 bzw. 5000 mg/kg zeigte ein Teil der
Tiere ein und zwei Tage nach der Substanzgabe verminderte
Aktivitaet; ab dem dritten Tag bis zum Ende der 14taegigen
Nachbeobachtung waren jedoch keine Unterschiede im
Vergleich zur Kontrolle mehr festzustellen. Es wurde keine
Mortalitaet beobachtet.
In der enzymatischen Studie wurde daher die Dosis von 5000
mg/kg eingesetzt. Die Enzymaktivitaeten wurden 24 Stunden
nach der Substanzgabe ermittelt. Hierbei zeigte sich eine
statistisch signifikante Inhibition der
Butyrylcholinesterase Aktivitaet um 98.1%; die beiden
anderen untersuchten Enzymaktivitaeten waren im Vergleich

zur Kontrolle unveraendert. Laut Angabe der Autoren zeigte die Testsubstanz daher keine Anzeichen fuer eine verzoegerte Neurotoxizitaet. Als Positivkontrolle wurde Tri-o-kresylphosphat mitgefuehrt.

Source: BASF AG Ludwigshafen

Test substance: Triisobutylphosphat

(90)

Type: Neurotoxicity

Remark: Es wurde die Auswirkung der Testsubstanz (keine Angabe ob n-Butyl-, Isobutyl- oder tert.Butylphosphat oder Gemisch) auf neurologische Parameter (Inhibition der neurotox. Esterase und der Acetylcholinesterase im Gehirn bzw. der Plasma-Butyrylcholinesterase) beim Huhn untersucht; die

Testsubstanz wurde im Abstand von 21 Tage zweimal oral appliziert. Es wurden insgesamt 20 Tiere eingesetzt, von denen 4 nach der ersten und zwei nach der zweiten Substanzgabe starben. 21 Tage nach der letzten Substanzgabe wurde das periphaere Nervensystem, das Rueckenmark und das Gehirn untersucht; verzoegerte Neurotoxizitaet wurde nicht festgestellt. Die Butyrylcholinesterase Aktivitaet war 24 Stunden nach der Substanzapplikation um Faktor 2-3 erhoeht; die beiden anderen Enzymaktivitaeten waren unveraendert.

Source: BASF AG Ludwigshafen

Test substance: Tributylphosphat, ohne weitere Angaben ob n-Butyl-, Isobutyl- oder tert. Butylphosphat bzw. Gemisch.

(71)

Type: Neurotoxicity

Remark: Es wurde die Auswirkung einer oralen Einzeldosis der Testsubstanz auf verschiedene Enzymaktivitaeten (neurotox. Esterase und Acetylcholinesterase im Gehirn, Butyrylcholinesterase im Plasma) beim Huhn untersucht. In einer vorab durchgefuehrten "range-finding" Studie wurde den Tieren die Testsubstanz in einem Dosisbereich zwischen 1000 und 5000 mg/kg verabreicht. In den beiden hoechsten Dosisgruppen von 4000 bzw. 5000 mg/kg zeigte ein Teil der Tiere ein und zwei Tage nach der Substanzgabe verminderte Aktivitaet; ab dem dritten Tag bis zum Ende der 14taegigen Nachbeobachtung waren jedoch keine Unterschiede im Vergleich zur Kontrolle mehr festzustellen. Es wurde keine Mortalitaet beobachtet.
In der enzymatischen Studie wurde daher die Dosis von 5000 mg/kg eingesetzt. Die Enzymaktivitaeten wurden 24 Stunden nach der Substanzgabe ermittelt. Hierbei zeigte sich eine statistisch signifikante Inhibition der

Butyrylcholinesterase Aktivitaet um 98.1%; die beiden anderen untersuchten Enzymaktivitaeten waren im Vergleich zur Kontrolle unveraendert. Laut Angabe der Autoren zeigte die Testsubstanz daher keine Anzeichen fuer eine verzoegerte Neurotoxizitaet. Als Positivkontrolle wurde Tri-o-kresylphosphat mitgefuehrt.

Source: BASF AG Ludwigshafen

Test substance: Triisobutylphosphat

(90)

Type: Neurotoxicity

Remark: Es wurde die Auswirkung der Testsubstanz (keine Angabe ob n-Butyl-, Isobutyl- oder tert.Butylphosphat oder Gemisch) auf neurologische Parameter (Inhibition der neurotox. Esterase und der Acetylcholinesterase im Gehirn bzw. der Plasma-Butyrylcholinesterase) beim Huhn untersucht; die Testsubstanz wurde im Abstand von 21 Tage zweimal oral appliziert. Es wurden insgesamt 20 Tiere eingesetzt, von denen 4 nach der ersten und zwei nach der zweiten

Substanzgabe starben. 21 Tage nach der letzten Substanzgabe wurde das periphaere Nervensystem, das Rueckenmark und das Gehirn untersucht; verzoegerte Neurotoxizitaet wurde nicht festgestellt. Die Butyrylcholinesterase Aktivitaet war 24 Stunden nach der Substanzapplikation um Faktor 2-3 erhoeht; die beiden anderen Enzymaktivitaeten waren unveraendert.

Source: BASF AG Ludwigshafen

Test substance: Tributylphosphat, ohne weitere Angaben ob n-Butyl-, Isobutyl- oder tert. Butylphosphat bzw. Gemisch.

(71)

Type: other: Review

Remark: Zusammenfassende Darstellungen

Source: BASF AG Ludwigshafen

Test substance: Triisobutylphosphat / Organophosphate

(91) (92)

Type: other: Review

Remark: Zusammenfassende Darstellungen

Source: BASF AG Ludwigshafen

Test substance: Triisobutylphosphat / Organophosphate

(93) (91) (92)

6.1 Analytical Methods
-

6.2 Detection and Identification
-

7.1 Function
-

7.2 Effects on Organisms to be Controlled
-

7.3 Organisms to be Protected
-

7.4 User
-

7.5 Resistance
-

8.1 Methods Handling and Storing

-

8.2 Fire Guidance

-

8.3 Emergency Measures

-

8.4 Possib. of Rendering Subst. Harmless
-

8.5 Waste Management
-

8.6 Side-effects Detection
-

8.7 Substance Registered as Dangerous for Ground Water
-

8.8 Reactivity Towards Container Material
-

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10.1 End Point Summary

-

10.2 Hazard Summary

-

10.3 Risk Assessment

-

201-16174B

RECEIVED
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IUCLID

Data Set

New Chemical	:	ID: 12645-31-7
CAS No.	:	12645-31-7
TSCA Name	:	2-ethylhexyl phosphate
Molecular Weight	:	210.21
Molecular Formula	:	C8 H19 O4 P1

Producer related part

Company	:	The Lubrizol Corporation
Creation date	:	04.03.2005

Substance related part

Company	:	The Lubrizol Corporation
Creation date	:	04.03.2005
Status	:	
Memo	:	
Printing date	:	17.10.2005
Revision date	:	
Date of last update	:	02.05.2005
Number of pages	:	30
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	American Chemistry Council (formerly Chemical Manufacturers Association) Phosphoric Acid Derivatives Panel
Contact person	:	
Date	:	
Street	:	Wilson Boulevard
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	703-741-5600
Telefax	:	703-741-6091
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : Bayer Corporation Pittsburgh
16.10.2001

Type	:	cooperating company
Name	:	Bayer Corporation
Contact person	:	
Date	:	
Street	:	
Town	:	
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : Bayer Corporation Pittsburgh
16.10.2001

Type	:	cooperating company
Name	:	Baker Petrolite Corporation
Contact person	:	
Date	:	
Street	:	
Town	:	
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : Bayer Corporation Pittsburgh
16.10.2001

Type	:	cooperating company
Name	:	Crompton Corporation
Contact person	:	
Date	:	
Street	:	

Town	:	
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : Bayer Corporation Pittsburgh
16.10.2001

Type	:	cooperating company
Name	:	ICI Americas (Uniqema)
Contact person	:	
Date	:	
Street	:	
Town	:	
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : Bayer Corporation Pittsburgh
16.10.2001

Type	:	cooperating company
Name	:	Noveon, Inc (formerly BF Goodrich)
Contact person	:	
Date	:	
Street	:	
Town	:	
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : Bayer Corporation Pittsburgh
16.10.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	< -20 °C
Sublimation	:	
Method	:	other: BS4633, OECD 102
Year	:	2005
GLP	:	yes
Test substance	:	other TS:2-ethylhexyl phosphate, purity: 39-51% CAS# 1070-03-7 (mono-2-ehp), 45-63% CAS# 298-07-7 (di-2-ehp)
Result	:	< 253 ± 0.5 degree K Temperature observations of the test material were recorded every 30 seconds. The determination was conducted in duplicate. Measured temperatures were converted from degrees C to degrees K using T=t+273.15. The test material became increasingly viscous during cooling.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

11.03.2005 (7)

2.2 BOILING POINT

Value	:	354.5 °C at 1013 hPa
Decomposition	:	
Method	:	other: MPBPWIN Program, version 1.31
Year	:	1999
GLP	:	no
Test substance	:	other TS: molecular structure
Result	:	Boiling Point: 354.51 deg C (Adapted Stein and Brown Method)
Source	:	Bayer Corporation Pittsburgh
Reliability	:	(2) valid with restrictions Accepted calculation method
Flag	:	Critical study for SIDS endpoint

22.10.2001 (4)

Value	:	> 93 °C at
Source	:	Bayer Corporation Pittsburgh

27.06.2001 (13)

Decomposition	:	yes
Method	:	
Year	:	
GLP	:	
Test substance	:	
Source	:	Bayer Corporation Pittsburgh

27.06.2001 (1)

2.3 DENSITY

Type	:	
Value	:	1.05 g/cm³ at 20 °C
Method	:	
Year	:	

GLP :
Test substance : other TS: 2-ethylhexyl phosphate; purity = 98%

Source : Bayer Corporation Pittsburgh
27.06.2001 (1)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .000000712 hPa at 25 °C
Decomposition :
Method : other (calculated): MPBPWIN Program, version 1.31
Year : 1999
GLP : no
Test substance : other TS: molecular structure

Result : Vapor Pressure Estimations (25 deg C):
(Using BP: 354.51 deg C (estimated))
(Using MP: 81.30 deg C (estimated))
VP: 1.9E-007 mm Hg (Antoine Method)
VP: 5.34E-007 mm Hg (Modified Grain Method)
VP: 5.7E-005 mm Hg (Mackay Method)
Selected VP: 5.34E-007 mm Hg (Modified Grain Method)
Source : Bayer Corporation Pittsburgh
Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
16.10.2001 (4)

Remark : nonvolatile
Source : Bayer Corporation Pittsburgh
27.06.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : 2.65 at °C
pH value :
Method : other (calculated): KOWWIN Program, version 1.65
Year : 1999
GLP : no
Test substance : other TS: molecular structure

Source : Bayer Corporation Pittsburgh
Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
10.03.2005 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : at 25 °C

pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	other: soluble
Stable	:	
Deg. product	:	
Method	:	OECD Guide-line 105
Year	:	2005
GLP	:	yes
Test substance	:	other TS:# 12645-31-7, is a mixture of mono(2-ethylhexyl) phosphate, CAS# 1070-03-7, (39-51%) and bis(2-ethylhexyl) phosphate, CAS# 298-07-7, (45-63%).
Method	:	Specialist Estimation Software WATERNET version 1.01 2000 U.S. Environmental Protection Agency and WSKOW v1.41 2000, US Environmental Protection Agency.
Remark	:	Mixtures of test material and glass double-distilled water were added to three separate flasks as follows:

Sample #	Mass of Test Material(g)	Volume of Water (ml)
1	0.1008	100
2	1.0118	100
3	5.0435	50

After addition of glass double-distilled water to the flasks, they were shaken at approximately 30°C for 17½ hours and, after standing at 20°C for a period 3¼ hours, the contents of the flasks were centrifuged at 13500 rpm for 35 minutes and filtered through 0.2 µm filters. The pH of each solution was measured. The concentration of test material in the sample solutions was determined by high performance liquid chromatography with mass selective detection (HPLC-MS). Duplicate aliquots (A and B) of the sample solution were diluted by factors of 500, 5000 and 50000 for samples 1, 2 and 3 respectively using acetonitrile. Duplicate standard solutions of test material were prepared in acetonitrile to cover a nominal concentration range of 0 to 10 mg/l.

The concentration (g/l) of the components within the test material in the sample solutions are shown in the following table:

Sample # / Time Shaken (g/l) at ~30°C(hrs)/ Time Equilibrated at 20°C (hrs0 / Concentration (g/l) monoester diester / Solution pH
1: 17½ / 3¼ / 0.437 / 3.99 x 10-3 / 2.7
2: 17½ / 3¼ / 2.23 / 1.88 x 10-2 / 2.2
3: 17½ / 3¼ / 1.62 / 0.103 / 2.0

The computer based estimate for the monoester component of the test material gave a WATERNT estimation of water solubility of 2.192 x 103 mg/l at 25°C. The diester component of the test material had an experimental water solubility database match using WSKOW v1.41 © 2000, U.S. Environmental Protection Agency. The water solubility was determined to be 182 mg/l at 25°C.

The software was validated with reference substances which had one or more functional groups present in the monoester component of the test material. The validation is shown in the following table:

Chemical Name / CAS No/ Experimentally Determined Water Solubility mg/l / Experimentally Determined Water Solubility Log10 mg / WSKOW Water Solubility mg/l / WSKOW Water Solubility Log10 mg/l
Ethane: 000074-84-0 / 60.2 / 1.78 / 383.29 / 2.58

Triethylphosphate: 000078-40-0 / 5 x 105 / 5.70 / 1.1525 x 105 / 5.06
2-Ethyl-1-hexanol: 000104-76-7 / 880 / 2.94 / 1285.3 / 3.11
1-Hexanol: 000111-27-3 / 5900 / 3.77 / 7135.9 / 3.85
Tributylphosphate: 000126-73-8 / 280 / 2.45 / 101.04 / 2.00

Since all software estimations were within +/- 1 log unit, and in the absence of any systematic errors, the software was considered valid for the estimation of the monoester component within the test material.

Result : 2.19x10^3 mg/l [mono(2-ethylhexyl) phosphate, CAS# 1070-03-7] 182 mg/l [bis(2-ethylhexyl) phosphate, CAS# 298-07-7]
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
09.03.2005 (12)

Solubility in :
Value : 211.3 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: WSKOW Program, version 1.36
Year : 1999
GLP : no
Test substance : other TS: molecular structure

Source : Bayer Corporation Pittsburgh
Reliability : (2) valid with restrictions
Accepted calculation method
16.10.2001 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1560000 molecule/cm³
Rate constant	:	.00000000328992 cm³/(molecule*sec)
Degradation	:	50 % after 3.9 hour(s)
Deg. product	:	
Method	:	other (calculated): AOP Program (v1.89)
Year	:	1999
GLP	:	no
Test substance	:	other TS: molecular structure
Result	:	-------- SUMMARY (AOP v1.89): HYDROXYL RADICALS -------- Hydrogen Abstraction = 32.6192 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 32.8992 E-12 cm3/molecule-sec HALF-LIFE = 0.325 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 3.901 Hrs
Source	:	Bayer Corporation Pittsburgh
Reliability	:	(2) valid with restrictions Accepted calculation method
Flag	:	Critical study for SIDS endpoint

27.06.2001 (4)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year	:	2005
GLP	:	yes
Test substance	:	other TS: 2-ethylhexyl phosphate , purity: 39-51% CAS# 1070-03-7 (mono-2-ehp), 45-63% CAS# 298-07-7 (di-2-ehp)
Remark	:	Assessment of hydrolytic stability was carried out using Method 111 of the OECD Guidelines for Testing of Chemicals, 12 May 1981. The results are as follows: with pH at Estimated half-life at 25°C (mono and diester components) 4 >1 year 7 >1 year 9 >1 year Sample solutions were prepared in stoppered glass flasks at a nominal concentration of 0.05 g/l in the three buffer solutions. A 1% co-solvent of

acetonitrile was used to aid solubility. The solutions were shielded from light whilst maintained at the test temperature. Sample solutions at pH 4, 7 and 9 were maintained at 50.0 ± 0.5°C for a period of 5 days. Aliquots of the sample solutions were taken from the flasks at various times and the pH of each solution recorded. The concentration of the sample solution was determined by high performance liquid chromatography (HPLC) with Mass Selective Detection (MSD). Duplicate aliquots (A and B) 5 ml of sample solution were diluted with 20 ml of water and then diluted to 50 ml with acetonitrile, in total by a factor of 10. Duplicate standard solutions of test material were prepared in relevant buffer*: acetonitrile (50:50 v/v) at a nominal concentration of 5 mg/l. The concentration of the sample solutions (g/l) was calculated using the HPLC peak areas of the sample and standard solutions.

Hydrodrolysis was less than 10% after 5 days at 50°C, equivalent to a half-life greater than 1 year at 25°C. The results were as follows:

pH 4 at 50 ± 0.5°C (monoester)
concetration at 0, 2.4, 25 and 120 hrs
Concentration (g/l): 5.08 x 10-2 / 4.97 x 10-2 / 5.10 x 10-2 /5.21 x 10-2
% of initial: - / 97.9 / 100 / 103

pH 4 at 50 ± 0.5°C (diester)
Concentration at 0, 2.4, 25, and 120 hrs
Concentration (g/l): 5.06 x 10-2 /4.85 x 10-2 / 4.97 x 10-2 /4.81 x 10-2
% of initial: - / 96.0 / 98.3 / 95.2

pH 7 at 50 ± 0.5°C (monoester)
Concentration at 0, 2.4, 25, and 120 hrs
Concentration (g/l): 5.06 x 10-2 / 5.02 x 10-2 / 5.20 x 10-2 /5.12 x 10-2
% of initial: - / 99.2 / 103 / 101

pH 7 at 50 ± 0.5°C (diester)
Concentration at 0, 2.4, 25, and 120 hrs
Concentration (g/l): 5.09 x 10-2 / 5.02 x 10-2 / 5.15 x 10-2 / 5.10 x 10-2
% of initial: - / 98.7 / 101 / 100

pH 9 at 50 ± 0.5°C (monoester)
Concentration at 0, 2.4, 25, and 120 hrs
Concentration (g/l): 5.07 x 10-2 / 5.09 x 10-2 / 5.08 x 10-2 / 5.14 x 10-2
% of initial: - / 100 / 100 / 101

pH 9 at 50 ± 0.5°C (diester)
Concentration at 0, 2.4, 25, and 120 hrs
Concentration (g/l): 5.10 x 10-2 / 5.06 x 10-2 / 5.11 x 10-2 / 5.12 x 10-2
% of initial: - / 99.1 / 100 / 100

Flag : Critical study for SIDS endpoint
02.05.2005 (7)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Level III Fugacity Model
Year :

Remark : Default input values of 1000 kg/hr were used for model.
Result : Media Concentration Half-Life Emissions Fugacity

	(percent)	(hr)	(kg/hr)	(atm)
Air	0.000783	7.8	1000	8.41e-015
Water	29	360	1000	1.65e-016
Soil	70.8	360	1000	9.56e-016
Sediment	0.188	1.44e+003	0	9.96e-017

Persistence Time: 452 hr
Reaction Time: 520 hr
Advection Time: 3.45e+003 hr
Percent Reacted: 86.9
Percent Advected: 13.1

Source : Bayer Corporation Pittsburgh
Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
10.03.2005 (4)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic, adapted
Concentration : 18.7 mg/l related to Test substance
10 mg/l related to COD (Chemical Oxygen Demand)
Contact time :
Degradation : 52 (±) % after 28 day(s)
Result : other:Not Ready Biodegradable
Deg. product :
Method : OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO_2 evolution)"
Year : 2004
GLP : yes
Test substance : other TS: 2-ethylhexyl phosphate , purity: 39-51% CAS# 1070-03-7 (mono-2-ehp), 45-63% CAS# 298-07-7 (di-2-ehp)

Method : Method C.4-C of Commission Directive 92/69/EEC (Annex V, Directive 67/548/EEC), and EPA OPPTS 835.3110
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

10.03.2005 (9)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species : other
Exposure period : at °C
Concentration :
BCF : 21.92
Elimination :
Method : other: BCF Program (v2.13)
Year :
GLP : no
Test substance : other TS: molecular structure

Result : CHEM : Phosphoric acid, 2-ethylhexyl ester
MOL FOR: C8 H19 O4 P1
MOL WT : 210.21
---------- Bcfwin v2.12 ----------
Log Kow (estimated) : 2.65
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 2.65

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction

Correction(s): Value
No Applicable Correction Factors

Estimated Log BCF = 1.341 (BCF = 21.92)
Source : Bayer Corporation Pittsburgh
Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
27.06.2001 (4)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	100
LC50	:	> 100
Limit test	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	2004
GLP	:	yes
Test substance	:	other TS: 2-ethylhexyl phosphate, purity: 39-51% CAS# 1070-03-7 (mono-2-ehp), 45-63% CAS# 298-07-7 (di-2-ehp)
Result	:	Following a preliminary range-finding test fish were exposed, in two groups of ten, to a single test concentration of 100 mg/l for a period of 96 hours at a temperature of approximately 14 C under semi-static test conditions. The test material solutions were prepared by stirring an excess (1000 mg/l) of test material in dechlorinated tap water using a magnetic stirrer for 23 hours. After the stirring period and a 1-Hour settlement period the saturated solution was removed by mid-depth siphon. A sample of the saturated solution was analysed for Total Organic Carbon (TOC) to determine the amount of test material present and the dilution required to give the 100 mg/l test concentration. The number of mortalities and any sub-lethal effects of exposure in each test and control vessel were determined 3 and 6 hours after the start of exposure and then daily throughout the test until termination after 96 hours. The 96-Hour LC50 based on nominal test concentrations was greater than 100 mg/l and correspondingly the No Observed Effect Concentration was 100 mg/l.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

11.03.2005 (8)

Type	:	static
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	>= 5018
Limit test	:	
Analytical monitoring	:	no
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS: Mixture of CAS# 1070-03-7 (mono-2-ehp), CAS# 298-07-7 (di-2-ehp), and CAS#128-39-2 (2,6 Di-t-butylphenol)
Remark	:	The test material was evaluated at concentrations of 0 ppm, 100 ppm, 499 ppm, 1026, ppm, 2026 ppm and 5018 ppm. The concentrations were prepared by adding the appropriate volumes of water and using a density of 0.935 g/ml to calculate the test concentrations. Twenty (20) fish were randomly assigned to each test chamber. The control chamber consisted of the same dilution water as for the test material. The fish were checked every 24 hours for mortality and abnormal behaviour. Dissolved oxygen and pH were also measure every 24 hours. Temperature was monitored continuously. LC50 values were calculated using an EPA (1978) computer software LC50 program. Dissolved oxygen remained above 60% saturation in all doses. pH values decreased slightly over time as test

material concentration increased. Insignificant mortality (1/20 fish) was observed in the control. The 96 hour LC50 was >5,018 ppm. No mortality was observed at 5,018 ppm. However, behaviour could not be monitored cloudiness due to the presence of the test material.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
11.03.2005 (6)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : 56
EC50 : 110
Analytical monitoring : yes
Method : OECD Guide-line 202
Year : 2004
GLP : yes
Test substance : other TS: 2-ethylhexyl phosphate , purity: 39-51% CAS# 1070-03-7 (mono-2-ehp), 45-63% CAS# 298-07-7 (di-2-ehp)

Result : Following a preliminary range-finding test and an initial experiment, twenty daphnids (2 replicates of 10) were exposed to test concentrations of 32, 56, 100, 180 and 320 mg/l for 48 hours at a temperature od approximately 21 °C under static test conditions. The test material solutions were prepared by stirring an excess (1000 mg.l) of test material in reconstituted water using a magnetic stirrer for 23 hours. After the stirring period and a 1-hour settlement period the saturated solution was removed by mid-depth siphon. A sample of the saturated solution was analysed by Total Organic Carbon (TOC) to determine the amount of test material present and the dilutions required to give the test series. The number of immobilized Daphnia were recorded after 24 and 48 hours. The 48-hour EC50 was 110 mg/l with 95% confidence limits of 93-120 mg/l. The No Observed Effect Level was 56 mg/l

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
10.03.2005 (8)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : growth rate
Exposure period : 72 hour(s)
Unit : mg/l
NOEC : 5
EC50 : 168
EC90 : 207
Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year : 1992
GLP : yes
Test substance : other TS: phosphoric acid, 2-ethylhexyl ester; purity not noted

Result : 24 hr EC50 = 110 mg/l
48 hr EC50 = 132 mg/l
Source : Bayer Corporation Pittsburgh
Test condition : test water: highly purified deionized water

		medium: OECD 201 recommended Freshwater Algal Assay medium pH: approx. 8 temperature: 21.2 - 23.1 degree C light: 8723, 9680, 8822 lux
Reliability	:	(1) valid without restriction GLP Giudeline study
16.10.2001		(2)

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	biomass
Exposure period	:	72 hour(s)
Unit	:	mg/l
NOEC	:	5
EC50	:	161
EC90	:	198
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	1992
GLP	:	yes
Test substance	:	other TS: phosphoric acid, 2-ethylhexyl ester; purity not noted
Result	:	24 hr EC50 = 110 mg/l 48 hr EC50 = 136 mg/l
Source	:	Bayer Corporation Pittsburgh
Test condition	:	test water: highly purified deionized water medium: OECD 201 recommended Freshwater Algal Assay medium pH: approx. 8 temperature: 21.2 - 23.1 degree C light: 8723, 9680, 8822 lux
Reliability	:	(1) valid without restriction GLP Giudeline study
Flag	:	Critical study for SIDS endpoint
16.10.2001		(2)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	500 - 1000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	female
Number of animals	:	9
Vehicle	:	
Doses	:	2000, 300 mg/kg bw
Method	:	OECD Guide-line 423
Year	:	
GLP	:	yes
Test substance	:	other TS: 2-ethylhexyl phosphate , purity: 39-51% CAS# 1070-03-7 (mono-2-ehp), 45-63% CAS# 298-07-7 (di-2-ehp)
Remark	:	The acute toxicity of the test material was studied using a single oral dose via gavage. A group of three fasted females was treated with the test material at a dose level of 2000 mg/kg bodyweight. Based on the results from this dose level further groups of fasted females were treated at a dose level of 300 mg/kg bodyweight. Dosing was performed sequentially as a single . The test material was administered orally undiluted for the 2000 mg/kg dose level and orally as a solution in arachis oil BP for the 300 mg/kg dose level. Groups of fasted animals were treated as follows:

Dose Level/ Specific Gravity /Concentration (mg/ml) / Dose Volume (ml/kg) / Number of Rats (Female)
2000: 1.013 / Not Applicable / 1.98 / 3
300: Not Applicable / 30 / 10 / 3
300: Not applicable / 30 / 10 / 3

The animals were observed for deaths or overt signs of toxicity ½, 1, 2 and 4 hours after dosing and subsequently once daily for up to fourteen days. Clinical signs and bodyweight development were monitored during the study. All animals were subjected to gross necropsy.
Two animals treated at a dose level of 2000 mg/kg were found dead one or two days after dosing. There were no deaths noted in animals treated at a dose level of 300 mg/kg. Signs of systemic toxicity noted in animals treated at a dose level of 2000 mg/kg were hunched posture, lethargy, piloerection, diarrhoea, diuresis, dehydration, ataxia, emaciation, decreased respiratory rate, laboured respiration and tiptoe gait. Primarily the effects noted were indicative of a strong gastric irritant and not a neurotoxicant. The macroscopic abnormalities noted at necropsy of the two moribund animals, treated at a dose level of 2000 mg/kg, also appeared to support this assessment; with epithelial sloughing and pale appearance of both the gastric mucosa and non-glandular region of the stomach. The effects noted in the animal that survived at a dose level of 2000 mg/kg, lethargy, piloerection, and diuresis (all at 4hr), hunched posture (4hrs and day 1), and tiptoe gait(day 1 and 2), were transient in nature and not due to neurotoxicity, as they were of relatively short duration and did not re-occur during the study period i.e. they were not intermittent. The fact that the effects seen in this surviving animal were considered to be transient would also indicate the test material to be a strong gastric irritant rather than a neurotoxicant. There was no indication that permanent damage to the

neural system was involved. The investigators noted that these types of findings were commonly observed on this type of study within this testing facility. The incidence and duration show no correlation with effects seen with known neurotxic materials. The surviving animal treated at a dose level of 2000 mg/kg appeared normal four days after dosing. There were no signs of systemic toxicity noted in animals treated at a dose level of 300 mg/kg. The surviving animals showed expected gains in bodyweight over the study period. Abnormalities noted at necropsy of animals that died during the study were haemorrhagic lungs, dark liver, dark kidneys, epithelial sloughing and pale gastric mucosa and epithelial sloughing and pale non-glandular region of the stomach. No abnormalities were noted at necropsy of animals that were killed at the end of the study. The acute oral median lethal dose (LD50) of the test material in the female Sprague Dawley CD strain rat was estimated to be in the range of 500 1000 mg/kg bodyweight.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
10.03.2005 (10)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type : other
Value :
Species :
Strain :
Sex :
Number of animals :
Vehicle :
Doses :

Remark : The dermal LD50 for tributyl phosphate and tris(2-ethyl hexyl) phosphate are > 10,000 mg/kg bw. It is predicted that the acute dermal toxicity of 2-ethyl hexyl phosphate will also be in the non-toxic range. (See IUCLID data sets on CAS#126-73-8 and 78-42-2)

09.03.2005

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Remark : Repeat dose studies have been conducted with other chemical members of the Phosphoric Acid Derivatives category, and demonstrate an apparent

reduction in toxicity with increasing molecular weight. The toxicity of 2-ethyl hexyl phosphate (12645-31-7) is expected to be similar to the toxicity of Dibutyl hydrogen phosphate (107-66-4) of same molecular weight. The 44 day oral exposure NOAEL of Dibutyl hydrogen phosphate is 30 mg/kg bw in rats. (See IUCLID data sets on surrogate chemicals 104-76-7, 149-57-5, 107-66-4 and 126-73-8, and 78-42-2.)

09.03.2005

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Bacterial reverse mutation assay
System of testing : Salmonella typhimurium strains TA1535, TA1537, TA98, TA100 and Escherichia coli strain WP2uvrA-
Test concentration : All Salmonella strains: 15, 50, 150, 500, 1500, 5000 µg/plate E.coli strain WP2uvrA-: 50, 150, 500, 1500, 5000 µg/plate
Cycotoxic concentr. : With metabolic activation: 5000 µg/plate to TA100. Without metabolic activation: 5000 µg/plate to TA100 Precipitation conc: Not noted at any concentration

Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 2004
GLP : yes
Test substance : other TS: 2-ethylhexyl phosphate , purity: 39-51% CAS# 1070-03-7 (mono-2-ehp), 45-63% CAS# 298-07-7 (di-2-ehp)

Method : The method conforms to the guidelines for bacterial mutagenicity testing published by the major Japanese Regulatory Authorities including METI, MHLW and MAFF. It also meets the requirements of Method B13/14 of Commission Directive 2000/32/EC and the USA, EPA (TSCA) OPPTS harmonised guidelines.
Remark : S. typhimurium strains TA1535, TA1537, TA98, TA100 and E. coli strain WP2uvrA- were treated with the test material using the Ames plate incorporation method at up to six dose levels, in triplicate, both with and without the addition of a rat liver homogenate metabolising system (10% liver S9 in standard co-factors). Vehicle and positive controls were used in parallel with the test material. A solvent treatment group was used as the vehicle control and the positive control materials used in the series of plates without S9-mix were as follows:
N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG): 3 µg/plate for TA100, 5 µg/plate for TA1535
and 2 µg/plate for WP2uvrA-
9-Aminoacridine (9AA): 80 µg/plate for TA1537
4-Nitroquinoline-1-oxide (4NQO): 0.2 µg/plate for TA98

In addition, 2-Aminoanthracene (2AA) and Benzo(a)pyrene (BP), which are non-mutagenic in the absence of metabolising enzymes, were used in the series of plates with S9-mix at the following concentrations:
2AA at 1 µg/plate for TA100
2AA at 2 µg/plate for TA1535 and TA1537
BP at 5 µg/plate for TA98
2AA at 10 µg/plate for WP2uvrA-
The dose range for the first experiment was determined in a preliminary toxicity assay and was 15 to 5000 and 50 to 5000 µg/plate for the Salmonella and E.coli strains respectively. The experiment was repeated on a separate day using the same dose range as Experiment 1, fresh cultures of the bacterial strains and fresh test material formulations.
An additional dose level was included (where applicable) to allow for test material induced toxicity, ensuring that a minimum of four non-toxic dose

levels were achieved.
The vehicle (dimethyl sulphoxide) control plates gave counts of revertant colonies within the normal range. All of the positive control chemicals used in the test induced marked increases in the frequency of revertant colonies, both with or without metabolic activation. Thus, the sensitivity of the assay and the efficacy of the S9-mix were validated.
The reverse mutation assay was considered valid if the following criteria were met:
1) All tester strain cultures exhibit a characteristic number of spontaneous revertants per plate in the vehicle and untreated controls.
2) The appropriate characteristics for each tester strain have been confirmed, eg rfa cell-wall mutation and pKM101 plasmid R-factor etc.
3) All tester strain cultures should be in the approximate range of 1 to 9.9 x 109 bacteria per ml.
4) Each mean positive control value should be at least two times the respective vehicle control value for each strain, thus demonstrating both the intrinsic sensitivity of the tester strains to mutagenic exposure and the integrity of the S9-mix.
5) There should be a minimum of four non-toxic test material dose levels.
6) There should be no evidence of excessive contamination.

The test material was considered positive if it induced a reproducible, dose-related and statistically (Dunnett's method of linear regression (5)) significant increase in the revertant count in at least one strain of bacteria.

The test material caused a visible reduction in the growth of the bacterial background lawn to all of the Salmonella strains both with and without S9 at 5000 µg/plate. No toxicity was noted to E.coli strain WP2uvrA-. The test material was, therefore, tested up to the maximum recommended dose level of 5000 µg/plate. No test material precipitate was observed on the plates at any of the doses tested in either the presence or absence of S9-mix.
No significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains, with any dose of the test material, either with or without metabolic activation. Therefore, the test material was considered to be non-mutagenic under the conditions of this test.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
10.03.2005 (11)

Type : Bacterial reverse mutation assay
System of testing : Salmonella typhimurium strains TA-1535, TA-1537, TA-1538, TA-98, TA-100 and Saccharomyces strain D4
Test concentration : 0.001 to 5.0 ug/plate
Cycotoxic concentr. : With metabolic activation: 5.0 ug/plate except for D4. Without metabolic activation: 5.0 ug/plate except for D4.

Metabolic activation : with and without
Result : negative
Method : other
Year : 1977
GLP : no data
Test substance : other TS:2-ethylhexyl phosphate , purity: 36% CAS# 1070-03-7 (mono-2-ehp), 50% CAS# 298-07-7 (di-2-ehp), 5% CAS# 7664-38-2, 5% 2-ethylhexanol

Method : According to Ames et al (1975), Mutation Res. 31:347-364; McCann et al. (1975) Proc. Nat. Acad. Sci. 72:5135-5139
Remark : The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation

preparations. Methylnitrosoquanidine, 2-nitrofluorene, and quinacrine mustard were used as the positive controls for non-activation; 2-anthramine, 2-acetylaminofluorene, and 8-aminoquinoline were used as positive controls for activiation. S-9 liver homogenates, which were prepared from Aroclor 1254-induced and noninduced adult Sprague-Dawley male rats as described by Ames et al (1975, were prepared from Binetics Laboratory Products, Litton Bionetics, Inc. An S-9 mix was prepared by adding the following ingredients per milliliter of mix: 4 µmoles NADP (sodium salt), 5 µmoles D-glucose-6-phosphate, 8 µmoles MgCL2, 33 µmoles KCL, 100 µmoles sodium phosphate buffer (pH 7.4), and 100 µl of rat liver S-9 fraction. Criteria which were used to determine whether a chemical was mutagenic were: 1) a positive dose response in revertants in strains TA-1535, TA-1537, TA-1538 over three concentrations with the lowest increase equal to twice the solvent control; 2) an positive dose response in revertants in strains TA-98 and TA-100 over three concentrations with the highest increase equal to twice the solvent control for TA-100 and 2-3 three times for TA-98 and D4; 3) and a pattern in starins from the same parental strain, and 4) reproducibility.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
11.03.2005 (3)

Type : Mammalian cell gene mutation assay
System of testing : L5178y/TK+/- mouse lymphoma cells
Test concentration : 1.0 µg/ml to 0.1 µg/ml
Cycotoxic concentr. : With metabolic activation: 1.0 µl/ml
Without metabolic activation: 1.0 µl/ml

Metabolic activation : with and without
Result : negative
Method : other
Year : 1983
GLP : yes
Test substance : other TS:2-ethylhexyl phosphate , purity: 36% CAS# 1070-03-7 (mono-2-ehp), 50% CAS# 298-07-7 (di-2-ehp), 5% CAS# 7664-38-2, 5% 2-ethylhexanol

Method : Clive et al., 1973, 1975, 1979; Gletten et al., 1975; Brown and Clive, 1978
Remark : The L5178y/TK+/- mouse lymphoma cells were obtained from Dr. Donald Clive, Bourroughs Wellcome and maintained in suspension culture. Cell populations were enumerated by fine particle analysis on a Particle Data Analyzer. S-9 mix prepared by the method of Getten et al., 1975, was purchased from Microbiological Associates, Rockville Maryland.

An initial toxicity assay was conducted to determine optimal dose levels. @-EHP was solubilizer in DSMO for dosing. Cultures were also dosed with positive (EMS for non-activated culture, DMBA for activated cultures) and negative (100 µl DMSO) controls. After 3 hours 2-EHP was removed by centrifugation and decanting the supernatant from the cultures and washing. The toxicity of 2-EHP was determined by cell population densities with the DMSO-treated control. The threshold level for complete toxicity was 1.0 µg/ml .

Based on the initial toxicity assay 2-EHP was tested over a range of concentrations from 1.0 µg/ml to 0.1 µg/ml. Repeat tests for non-activated and activated were conducted over narrower ranges of 0.32 µg/ml to 0.1 µg/ml and 0.20 µg/ml to 0.07 µg/ml, respectively. The activation assay was repeated a second time because of high mutation frequency in the DMSO-control. Total growth ranged from 0.8% to 78.7% (of the DMSO-treated controls) for the non-activated cultures and from 4.8% to 104.1% for activated cultures. The total growth and suspension growth of both non-activated and activated cultures was clearly dependent on 2-EHP

concentration. None of the clonable cultures treated with 2-EHP without and with activation exhibited mutation frequencies which were significantly different from the average mutant frequencies of the DMSO-control.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
11.03.2005 (5)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : other
Species :
Sex :
Strain :
Route of admin. :
Exposure period :
Doses :
Result :
Method :
Year :
GLP :
Test substance :

Remark : Chromosomal aberration assays have been negative with 2-ethylhexanol in rats(104-76-7), dibutyl hydrogen phosphate in mice (107-66-4), and tributyl phosphate in rats (126-73-8).i

09.03.2005

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : other
Sex :
Strain :
Route of admin. :
Exposure period :
Frequency of treatm. :
Duration of test :
Doses :
Control group :

Remark : Adequate developmental studies are available for surrogate chemicals 104-76-7, 149-57-5, 107-66-4 and 126-73-8.

09.03.2005

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type : other
In vitro/in vivo :
Species :
Sex :
Strain :

Route of admin.	:	
Exposure period	:	
Frequency of treatm.	:	
Duration of test	:	
Doses	:	
Control group	:	
Remark	:	Adequate reproductive studies are available for surrogate chemicals 104-76-7, 149-57-5, 107-66-4 and 126-73-8.

09.03.2005

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

9. References

(1) Crompton MSDS

(2) Environmental Services Group, Baker Petrolite Corporation, Missouri, USA. April, 2001.

(3) Litton Bionetics, Inc., Sponsored by Mobil Chemical Corp., 1977, EPA/OTS 0528761

(4) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510

(5) Mobil Environmental and Health Science Laboratory, Plainsboro, NJ, January 4, 1983.

(6) Mobil Oil Corp., 1991 , EPA/OTS #0536290

(7) SafePharm Laboratories, Derbyshire, UK, sponsored by The Lubrizol Corporation, February 28, 2005.

(8) SafePharm Laboratories, Derbyshire, UK, sponsored by The Lubrizol Corporation, November 1, 2004.

(9) SafePharm Laboratories, Derbyshire, UK, sponsored by The Lubrizol Corporation, October 26, 2004.

(10) SafePharm Laboratories, Derbyshire, UK, sponsored by The Lubrizol Corporation, October 5, 2004.

(11) SafePharm Laboratories, Derbyshire, UK, sponsored by The Lubrizol Corporation, September 13, 2004.

(12) SafePharm Laboratories, Derbyshire, UK, sponsored by The Lubrizol Corporation, September 28, 2004.

(13) Uniqema data

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

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I U C L I D

D a t a S e t

Existing Chemical	ID: 107-66-4
CAS No.	107-66-4
EINECS Name	dibutyl hydrogen phosphate
EINECS No.	203-509-8
TSCA Name	Phosphoric acid, dibutyl ester
Molecular Formula	C8H19O4P

Producer Related Part
Company:
Creation date: 21-JAN-1994

Substance Related Part
Company:
Creation date: 21-JAN-1994

Memo: Data for Phosphoric Acid Derivatives Category

Printing date:	29-JUN-2001
Revision date:	14-FEB-1994
Date of last Update:	14-FEB-2000

Number of Pages: 18

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information
-

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: inorganic
Physical status: liquid

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

DI-N-BUTYL PHOSPHATE

DIBUTYL HYDROGEN PHOSPHATE

DIBUTYL PHOSPHATE

PHOSPHORIC ACID, DIBUTYL ESTER

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity

Quantity

1.6.1 Labelling

1.6.2 Classification

1.7 Use Pattern

Type:	type
Category:	Non dispersive use
Type:	industrial
Category:	Chemical industry: used in synthesis
Type:	use
Category:	Intermediates

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution

1.14.2 Major Accident Hazards

1.14.3 Air Pollution

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value: ca. -13 degree C

(1)

2.2 Boiling Point

Value: > 200 degree C at 20 hPa
Decomposition: yes

(1)

2.3 Density

Type: density
Value: 1.05 g/cm3 at 20 degree C

(1)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: < .1 hPa at 20 degree C

(1)

2.5 Partition Coefficient

log Pow: .6 - 1.4
Method: other (calculated): Leo, A.: CLOGP-3.54 MedChem Software 1989. Daylight, Chemical Information Systems, Claremont, CA 91711, USA
Year:

(2)

log Pow: 2.2889
Method: other (calculated): KOWWIN Program, version 1.65
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure

(16)

2.6.1 Water Solubility

Value: 18 g/l at 20 degree C

(1)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: 188 degree C
Type: other
Method: other: DIN 51376
Year:

(1)

2.8 Auto Flammability

-

2.9 Flammability

-

2.10 Explosive Properties

-

2.11 Oxidizing Properties

-

2.12 Additional Remarks

Remark: pK value: 1.17

(3)

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: 52.6999 E-12 cm3/(molecule * sec)
Degradation: 50 % after 2.436 hour(s)
Method: other (calculated): AOP Program (v1.89)
Year: 1999 GLP: no
Test substance: other TS: molecular structure

(16)

3.1.2 Stability in Water

-

3.1.3 Stability in Soil

-

3.2 Monitoring Data (Environment)

-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - water - soil - sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: Level III Fugacity Model
Year:
Result:

Media	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.183	4.87	1000	1.58e-012
Water	34.4	208	1000	2.65e-014
Soil	65.3	208	1000	2.52e-013
Sediment	0.112	832	0	1.48e-014

Persistence Time: 253 hr
Reaction Time: 279 hr
Advection Time: 2.76e+003 hr
Percent Reacted: 90.8
Percent Advected: 9.2

Remark: Default input values of 1000 kg/hr were used for model.

(16)

3.3.2 Distribution

-

3.4 Mode of Degradation in Actual Use

-

3.5 Biodegradation

Type:
Inoculum: predominantly domestic sewage
Concentration: 4.4 mg/l
Degradation: 12 % after 28 day
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: GLP:
Test substance:
Remark: related to BOD

(4)

Type:
Inoculum:

7 day	9 %
14 day	97 %
21 day	> 98 %
28 day	> 98 %

Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: GLP:
Test substance:

(4)

3.6 BOD5, COD or BOD5/COD Ratio

-

3.7 Bioaccumulation

-

3.8 Additional Remarks

-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type:
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC0: >= 100
Method: other: Akute Toxizitaet fuer Fische (C.1.), Richtlinie 67/548/EWG (Entwurf 1992)
Year: GLP:
Test substance:

(4)

Type:
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC0: > 10000
Method: other: Letale Wirkung beim Zebrabaerbling, UBA-Verfahrensvorschlag, Mai 1984, Letale Wirkung beim Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h
Year: GLP:
Test substance:
Remark: direct weight

(4)

Type: other: calculation
Species: other: fish
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 83.187
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure

(16)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: other: calculation
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
LC50 : 90.941
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure

(16)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: green algae
Endpoint:
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 57.811
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure

(16)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring:
EC50: > 10000
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: GLP:
Test substance:
Remark: direct weight

(4)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 3200 mg/kg bw
Method:
Year: GLP:
Test substance:

(5)

Type: LD50
Species: rat
Strain:
Sex: male/female
Number of Animals: 5
Vehicle: no data
Value: > 2000 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: GLP: yes
Test substance: other TS
Test substance: purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%
15-APR-1999 (6)

5.1.2 Acute Inhalation Toxicity

-

5.1.3 Acute Dermal Toxicity

-

5.1.4 Acute Toxicity, other Routes

-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: highly irritating
EC classificat.:
Method: other: see remarks
Year: GLP:
Test substance:
Remark: method: ear, exposure time: 8 h, dose: 500 ul/animal, semi-occlusive, postexposure observation period: 7 d

(7)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: highly irritating
EC classificat.:
Method: other: see remarks
Year: GLP:
Test substance:
Remark: method: dose: 100 ul/animal, postexposure observation period: 7 d
test substance causes corrosion of the cornea

(7)

5.3 Sensitization

Type:	Guinea pig maximization test			
Species:	guinea pig			
Concentration:	Induction	1	%	intracutaneous
	Induction	10	%	occlusive epicutaneous
	Challenge	2	%	occlusive epicutaneous
Number of Animals:	10			
Vehicle:	water			
Result:	not sensitizing			
Classification:				
Method:	OECD Guide-line 406 "Skin Sensitization"			
Year:	1999		GLP: yes	
Test substance:	other TS: purity 99,4%			
Remark:	5 animals in control group			

14-FEB-2000 (8)

5.4 Repeated Dose Toxicity

Species:	rat Sex: male/female
Strain:	Sprague-Dawley
Route of admin.:	gavage
Exposure period:	44 days (male) and from 14 days before mating to day 3 of lactation (females)
Frequency of treatment:	daily
Post. obs. period:	no
Doses:	0, 30, 100, 300 and 1000 mg/kg
Control Group:	yes
NOAEL:	30 mg/kg bw
Method:	other
Year:	1995 GLP: yes
Test substance:	other TS
Method:	OECD Guideline 422
Remark:	Number of animals: 10/sex/group; Vehicle: sesame oil
Result:	transient red urine and a decrease in food consumption with >= 100 mg/kg (males). 3 males and 2 females died in the 1000 mg/kg-group. No effects on urinary, hematological and blood chemical findings in the males (females not given). Histopathology showed epithelial hyperplasia accompanied by degeneration and ulceration of the urinary bladder mucosa in males and females with >= 100 mg/kg. Epithelial hyperplasia and hyperkeratosis of the forestomach (some with erosion and ulceration in the gastric mucosa) were noted in both sexes >= 300 mg/kg. Increase of absolute and relative liver weight and hepatocellular swelling in females with 1000 mg/kg. NOEL 30 mg/kg bw. For reproductive effects see 5.8.
Test substance:	purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%

15-APR-1999 (6)

Species: hen Sex: no data
Strain: no data
Route of admin.: dermal
Exposure period: 90 d
Frequency of treatment:
Post. obs. period: no data
Doses: 100 mg/kg bw/d
Control Group: no data specified
Method:
Year: GLP:
Test substance:
Remark: purity not known
Result: delayed neurotoxic effects (no details, no further data)
(9)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: S. typhimurium TA100, TA1535, TA98, TA1537, E.coli WP2uvrA
Concentration: 0 - 156.2 µg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1995 GLP: yes
Test substance: other TS
Method: Guideline for Screening Mutagenicity Testing of Chemicals (Japan)
Remark: plate incorporation assay, vehicle acetone, toxicity was observed with 156.2 µg/plate
Test substance: purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%
15-APR-1999
(6)

Type: Ames test
System of testing: S. typhimurium TA 1535, TA 1537, TA 98, TA 100
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
(10)

Type: Cytogenetic assay
System of testing: Chinese hamster CHL/IU cells
Concentration: 0 - 0.54 mg/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1995 GLP: yes
Test substance: other TS
Method: Guideline for Screening Mutagenicity Testing of Chemicals (Japan)
Remark: no clastogenicity, no polyploidy, tested up to 50% growth inhibition
Test substance: purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%
16-APR-1999 (6)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse Sex: male/female
Strain: NMRI
Route of admin.: gavage
Exposure period: twice at an interval of 24 hours
Doses: 0, 100, 300, 1000 mg/kg bw
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: 1999 GLP: yes
Test substance: other TS: purity 99,4%
Remark: Number of animals: 5/sex/group; vehicle: deionized water
Result: 1000mg/kg bw caused death in 2 females with macroscopic findings of orange spume in gastro-intestinal tract; these 2 females were replaced and survived after treatment; motor activity was decreased in group 1000mg/kg bw; ratio of polychromatic erythrocytes to total erythrocytes was not changed to a significant extent
14-FEB-2000 (11)

5.7 Carcinogenicity
-

5.8 Toxicity to Reproduction

Type: other
Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure Period: 44 days (male) and from 14 days before mating to day 3 of lactation (females)
Frequency of treatment: daily
Duration of test:
Doses: 0, 30, 100, 300 and 1000 mg/kg
Control Group: yes
Method: other
Year: 1995 GLP: yes
Test substance: other TS
Method: OECD Guideline 422
Remark: Number of animals: 10/sex/group; Vehicle: sesame oil
Result: transient red urine and a decrease in food consumption with >= 100 mg/kg (males). 3 males and 2 females died in the 1000 mg/kg-group. Epithelial hyperplasia accompanied by degeneration and ulceration of the urinary bladder mucosa in males and females with >= 100 mg/kg. Epithelial hyperplasia and hyperkeratosis of the forestomach (some with erosion and ulceration in the gastric mucosa) were noted in both sexes >= 300 mg/kg. Increase of absolute and relative liver weight and hepatocellular swelling in females with 1000 mg/kg. No significant effects on reproductive parameters including copulation index, fertility index, number of corpora lutea and implantation sites, gestation index and gestation length. The number of live pubs and the viability index decreased with 1000 mg/kg, attributable to the high incidence of fatalities of pubs in some litters at or after birth.
Test substance: purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%

15-APR-1999 (6)

5.9 Developmental Toxicity/Teratogenicity

-

5.10 Other Relevant Information

Type: Metabolism
Remark: rat, single i.p. infection of 250 mg/kg:
only 0.072 and 0.023 % of the applied dose was found in the urine as S-containing metabolites.

(12)

Type:
Remark: Metabolism:
after i.p.-administration of the pesticide aminophon (O,O-di- n-butyl-1-n-butyl-amino-cyclohexyl-phosphonate) to rats, dibutylphosphate was detectable in the urine among other metabolites; orally administered aminophon also yielded dibutylphosphate, but to a lesser amount, in the urine.

(13)

Type:
Remark: Metabolism:
after a single i.p.-administration of tributyl phosphate at a dose of 250 mg/kg bw to male rats, dibutyl phosphate was identifiable in the 24-h urine among other phosphorus-containing metabolites. When rats were dosed with dibutyl phosphate, 47.6 % was recovered intact in the urine.

(14)

Type:
Remark: Metabolism:
in vitro-study: prolonged incubation of tributylphosphate with rat liver 9000 g supernatant: dibutylphosphate was detectable among other metabolites (amount of dibutylphosphate: 3 % of the applied substrate=tributylphosphate).

(15)

5.11 Experience with Human Exposure

Remark: workers exposed to unspecified concentrations of vapor complained of respiratory irritation and headache (no further data).

(5)

(1) Safety Data Sheet Bayer AG 24.02.1992

(2) Calculation UWS-Produktsicherheit, Bayer AG 1991

(3) Dyrssen, Acta Chem. cand. 11, 1771 (1957)

(4) Bayer AG data

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(6) Ministry of Health and Welfare Japan, Toxicity Testing Reports of Environmental Chemicals Vol. 2, 55- 78, 1995 (ISSN 1340-3842)

(7) Thyssen, J.: Bayer AG data, short report, 1.9.1978

(8) Seeberger, A.: Unpublished report of Hoechst Marion Roussel GmbH, No. 99.0099, June 2, 1999

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(10) Poth, A.: data of the CCR Project 156802, Report No. R 4872: Salmonella typhimurium reverse mutation assay with Phosphoric acid, dibutylester, 7.11.1989 (at the request of Bayer AG)

(11) Stammberger, I.: unpublished report of Hoechst Marion Roussel GmbH, No. 99.0313, August 26, 1999

(12) Suzuki, T. et al.: J. Agric. Food Chem. 32, 1278-1283 (1984)

(13) Riemer, F. et al.: 221-224: in Industrial and Environmental Xe- nobiotics, In Vitro Versus In Vivo Biotransformation and Toxici- ty, ed. Fouts, J.R. and Gut, I., Excerpta Medica, Amsterdam (1978)

(14) Suzuki, T. et al.: J. Agric. Food Chem. 32, 603-610 (1984)

(15) Sasaki, K. et al.: Bull. Environ. Contam. Toxicol. 33, 281-288 (1984)

(16) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510

7. Risk Assessment

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

201-16174B

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Data Set

Existing Chemical	:	ID: 1070-03-7
CAS No.	:	1070-03-7
IUPAC Name	:	phosphoric acid, mono(2-ethylhexyl) ester
Molecular Formula	:	C8H19O4P1
Molecular Weight	:	210.12

Producer related part

Company	:	The Lubrizol Corporation
Creation date	:	10.03.2005

Substance related part

Company	:	The Lubrizol Corporation
Creation date	:	10.03.2005
Status	:	
Memo	:	
Printing date	:	14.12.2005
Revision date	:	
Date of last update	:	04.04.2005
Number of pages	:	21
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	American Chemistry Council
Contact person	:	
Date	:	
Street	:	1300 Wilson Boulevard
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

10.03.2005

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name	:	phosphoric acid, mono(2ethylhexyl) ester
Smiles Code	:	
Molecular formula	:	C8H19O4P1
Molecular weight	:	210.12
Petrol class	:	

10.03.2005

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

10.03.2005

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

2.2 BOILING POINT

Value	:	354.5 °C at 1013 hPa
Decomposition	:	yes
Method	:	other:MPBPWIN Program, version 1.31
Year	:	1999
GLP	:	no
Test substance	:	other TS: molecular structure
Result	:	Boiling Point: 354.51 deg C (Adapted Stein and Brown Method)
Reliability	:	(2) valid with restrictions Accepted calculation method
Flag	:	Critical study for SIDS endpoint

11.03.2005 (3)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.000000534 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated):EPI Suite v3.10 Copyright 2000.
Year	:	
GLP	:	
Test substance	:	
Reliability	:	(2) valid with restrictions Accepted calculation method
Flag	:	Critical study for SIDS endpoint

11.03.2005 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	2.65 at °C
pH value	:	
Method	:	other (calculated): KOWWIN Program, version 1.65
Year	:	1999
GLP	:	no
Test substance	:	other TS: molecular structure
Reliability	:	(2) valid with restrictions Accepted calculation method
Flag	:	Critical study for SIDS endpoint

11.03.2005 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	211 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: WSKOW Program, version 1.36
Year	:	1999
GLP	:	no
Test substance	:	other TS: molecular structure
Reliability	:	(2) valid with restrictions Accepted calculation method
Flag	:	Critical study for SIDS endpoint

11.03.2005 (3)

Solubility in	:	Water
Value	:	at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	other:soluble
Stable	:	
Deg. product	:	
Method	:	OECD Guide-line 105
Year	:	2005
GLP	:	yes
Test substance	:	other TS:2-ethylhexyl phosphate, purity : 39-51% cas# 1070-03-7 (mono-2-ehp), 45-63% cas# 298-07-7 (di-2-ehp)
Method	:	Specialist Estimation Software WATERNET version 1.01 2000 U.S. Environmental Protection Agency and WSKOW v1.41 2000, US Environmental Protection Agency.
Remark	:	Mixtures of test material and glass double-distilled water were added to three separate flasks as follows:

Sample #	Mass of Test Material(g)	Volume of Water (ml)
1	0.1008	100
2	1.0118	100
3	5.0435	50

After addition of glass double-distilled water to the flasks, they were shaken at approximately 30°C for 17½ hours and, after standing at 20°C for a period 3¼ hours, the contents of the flasks were centrifuged at 13500 rpm for 35 minutes and filtered through 0.2 μm filters. The pH of each solution was measured. The concentration of test material in the sample solutions was determined by high performance liquid chromatography with mass selective detection (HPLC-MS). Duplicate aliquots (A and B) of the sample solution were diluted by factors of 500, 5000 and 50000 for samples 1, 2 and 3 respectively using acetonitrile. Duplicate standard solutions of test material were prepared in acetonitrile to cover a nominal concentration range of 0 to 10 mg/l.

The concentration (g/l) of the components within the test material in the sample solutions are shown in the following table:

Sample # / Time Shaken (g/l) at ~30ºC(hrs)/ Time Equilibrated at 20ºC (hrs0 / Concentration (g/l) monoester diester / Solution pH
1: 17½ / 3¼ / 0.437 / 3.99 x 10-3 / 2.7
2: 17½ / 3¼ / 2.23 / 1.88 x 10-2 / 2.2
3: 17½ / 3¼ / 1.62 / 0.103 / 2.0

The computer based estimate for the monoester component of the test material gave a WATERNT estimation of water solubility of 2.192 x 103 mg/l at 25°C. The diester component of the test material had an experimental water solubility database match using WSKOW v1.41 © 2000, U.S. Environmental Protection Agency. The water solubility was determined to be 182 mg/l at 25°C.

The software was validated with reference substances which had one or more functional groups present in the monoester component of the test material. The validation is shown in the following table:

Chemical Name / CAS No/ Experimentally Determined Water Solubility mg/l / Experimentally Determined Water Solubility Log10 mg / WSKOW Water Solubility mg/l / WSKOW Water Solubility Log10 mg/l
Ethane: 000074-84-0 / 60.2 / 1.78 / 383.29 / 2.58
Triethylphosphate: 000078-40-0 / 5 x 105 / 5.70 / 1.1525 x 105 / 5.06
2-Ethyl-1-hexanol: 000104-76-7 / 880 / 2.94 / 1285.3 / 3.11
1-Hexanol: 000111-27-3 / 5900 / 3.77 / 7135.9 / 3.85
Tributylphosphate: 000126-73-8 / 280 / 2.45 / 101.04 / 2.00

Since all software estimations were within +/- 1 log unit, and in the absence of any systematic errors, the software was considered valid for the estimation of the monoester component within the test material.

Result : 2.19x103 mg/l [mono(2-ethylhexyl) phosphate, CAS# 1070-03-7]
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
04.04.2005 (6)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
DIRECT PHOTOLYSIS		
Halflife t1/2	:	3.9 hour(s)
Degradation	:	% after
Quantum yield	:	
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1560000 molecule/cm^3
Rate constant	:	.00000000328992 cm^3/(molecule*sec)
Degradation	:	50 % after 3.9 hour(s)
Deg. product	:	
Method	:	other (calculated): AOP Program (v1.89)
Year	:	1999
GLP	:	no
Test substance	:	other TS: molecular structure
Result	:	----------Summary (AOP v1.89): HYDROXYL RADICALS-------- Hydrogen Abstraction = 32.6192 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 32.8992 E-12 cm3/molecule-sec HALF-LIFE =0.325 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE =3.901 Hrs
Reliability	:	(2) valid with restrictions Accepted calculation method
Flag	:	Critical study for SIDS endpoint

11.03.2005 (3)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)

Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Level III Fugacity Model
Year :

Remark : Default input values of 1000 kg/hr were used for model.
Result : Media Concentration Half-Life Emissions Fugacity

	(percent)	(hr)	(kg/hr)	(atm)
Air	0.000783	7.8	1000	8.41e-015
Water	29	360	1000	1.65e-016
Soil	70.8	360	1000	9.56e-016
Sediment	0.188	1.44e+003	0	9.96e-017

Persistence Time: 452 hr
Reaction Time: 520 hr
Advection Time: 3.45e+003 hr
Percent Reacted: 86.9
Percent Advected: 13.1

Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
11.03.2005

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	2710 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	
Number of animals	:	20
Vehicle	:	
Doses	:	464, 1000, 2150, 4640
Method	:	
Year	:	1971
GLP	:	no
Test substance	:	other TS: mono(2-ethylhexyl) phosphate, purity:unknown
Remark	:	The undiluted test material was fed via gavage to groups of rats (5/group) at 464 mg/kg, 1000 mg/kg, 2150 mg/kg, and 4640 mg/kg. The LD50 was determined to be 2710 mg/kg with lower and upper confidence limits of 2000-3690 mg/kg. The no observed effect level was 1000 mg/kg. Higher doses produced acute depression, excessive urination and diarrhea. Necrotic tissue in the stomach was observed in animals that survided 2150 mg/kg. The study was terminated at 14 days following treatment.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

11.03.2005 (1)

Type	:	LD50
Value	:	4100 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1970
GLP	:	no
Test substance	:	other TS:mono(2-ethylhexyl) phosphate, purity:unknown
Remark	:	The undiluted test material was fed via gavage to groups of male and female rats with a male to female ratio of 2/3 at 2000 mg/kg, 3/2 at 3160 mg/kg, 2/3 at 5010 mg/kg, and 3/2 at 7940 mg/kg. The LD50 was determined to be 4100 mg/kg with lower and upper confidence limits of 3530-4760 mg/kg. No deaths were observed at 2000 mg/kg. Toxic signs included reduced appetite, and activity, increasing weakness, collapse and death. Gross pathological observation included lung hyperemia, liver discoloration, and gastrointestinal inflammation. All surviving animals were sacrificed after 7 days.
Reliability	:	(2) valid with restrictions

11.03.2005 (7)

Type	:	LDLo
Value	:	3645 mg/kg bw
Species	:	rat
Strain	:	no data

Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1947
GLP	:	no
Test substance	:	
Remark	:	The undiluted test material was fed via gavage to 3 rats. The rat dosed with 2304 mg/kg exhibited nervousness on day 1 and weight loss on day 3 post exposure. No gross pathologic abnormalities were found. The rat dosed with 3645 mg/kg exhibited nervousness on day 1 and weight loss on day 2 post exposure. Gastrointestinal irritation was found upon sacrifice at day 9. The rat dosed with 6114 mg/kg died within 19 hours of treatment. Hemorrhagic areas were noted in the stomach. Small Intestines were distended with blood. The surface of the stomach and spleen next to the stomach was gray.
Reliability	:	(3) invalid

11.03.2005 (2)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 4640
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1971
GLP	:	no
Test substance	:	other TS: mono(2-ethylhexyl) phosphate, purity: unknown
Remark	:	The undiluted test material was applied to the clipped intact skin of four rabbits at dose of 4640 mg/kg. No deaths or systemic toxicity were observed. Severe erythema and edema was observed (corrosive).
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

10.03.2005 (1)

Type	:	LDLo
Value	:	1260 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	
Vehicle	:	
Doses	:	794, 1260, 2000, 3160
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: mono(2-ethylhexyl) phosphate, purity: unknown

Remark : The undiluted test material was applied to the clipped intact skin of rabbits at dose of 794 mg/kg (1 male), 1260 mg/kg (1 male AND 2 females), 2000 mg/k (2 males and 1 female), and 3160 mg/kg (1 female). No deaths occurred at 1260 mg/kg; one out of three animals died at 2000 mg/kg. Toxic signs included reduced appetite, and activity, lethargy, increasing weakness, collapse and death. Gross pathological observation included lung hyperemia, liver discoloration, enlarged gall bladder and slight gastrointestinal inflammation. All surviving animals were sacrificed after 14 days.

Reliability : (2) valid with restrictions

11.03.2005 (7)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : corrosive
Classification :
Method : other: Company Standard Method
Year : 1982
GLP : no data
Test substance : other TS: mono(2-ethylhexyl) phosphate, purity: unknown

Remark : The test material was applied to the clipped intact skin of 3 albino rabbits and covered with plastic strips. The sites were evaluated at 4, 24, 48, 72, 120, and 168 hours accoriding to Draize (1944). The compound was classified as a corrosive. The average maximum score was 8.0 out of 8 in 24 hours. No change was observed at termination (168 hours.

Reliability : (2) valid with restrictions

11.03.2005 (5)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals : 3
Vehicle :
PDII :
Result : corrosive
Classification :
Method :
Year : 1970
GLP : no
Test substance : other TS: mono(2-ethylhexyl) phosphate, purity: unknown

Remark : The test material was applied to the clipped intact skin of 3 albino rabbits and covered with plastic strips. The sites were evaluated at 4, 24, 48, 72, 120, and 168 hours accoriding to Draize (1944). The compound was classified as a corrosive. The average maximum score was 8.0 out of 8 in 24 hours. No change was observed at termination (168 hours.

Reliability : (2) valid with restrictions

11.03.2005 (7)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	3
Vehicle	:	
Result	:	corrosive
Classification	:	
Method	:	other: Company Standard Method
Year	:	1981
GLP	:	no data
Test substance	:	other TS: mono(2-ethylhexyl) phosphate, purity unknown
Remark	:	The test material (0.01 ml) was instilled into one eye of each of the 3 rabbits. Evaluations at 1, 24, 48, and 72 hours after treatment found that the average irritation scores were 51.4, 66, 77.9 and 68.3, respectively. The corneal opacity did not improve within 10 days suggesting possible irreversible/corrosive effects.
Reliability	:	(2) valid with restrictions

11.03.2005 (4)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	
Result	:	corrosive
Classification	:	
Method	:	
Year	:	1970
GLP	:	no
Test substance	:	other TS: mono(2-ethylhexyl) phosphate, purity unknown
Remark	:	The test material (0.01 ml) was instilled into one eye of each of the six rabbits. The eyes remained unwashed. Evaluations were made at 1, 24, 48, 72, 120, and 168 hours according to the method of Draize (1944). The average irritation score was 83.3 out of 110 at 24 hours. The compound was classified as a severe irritant to corrosive. At 240 hours opalescent areas of corneal cloudiness were still present with iris hemorrhagic and showing reaction to light.
Reliability	:	(2) valid with restrictions

11.03.2005 (7)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	3
Vehicle	:	
Result	:	corrosive
Classification	:	
Method	:	other: 21 CFR 191.12

Year	:	1971
GLP	:	no data
Test substance	:	other TS: mono(2-ethylhexyl) phosphate, purity unknown
Remark	:	The test material (0.01 ml) was instilled into one eye of each of the 3 rabbits. Evaluations were made at 24, 48, and 72 hours after treatment using the "Illustrate Guide for Grading Eye Irritation by Hazardous Substances". Erythema and edema of the cornea and moderate opacity were observed. The mean high score at 24 hours was 24 out of 110. The irritating effects were remised in 5-7 days.
Reliability	:	(2) valid with restrictions

11.03.2005 (1)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

9. References

(1) Akzo (1971), EPA/OTS #0530288

(2) E. I. DuPont De Nemours & Co. (1947), EPA/OTS #0530139

(3) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510

(4) Mobil Oil Corp., 1981 , EPA/OTS #0530435

(5) Mobil Oil Corp., 1982 , EPA/OTS #0530435

(6) SafePharm Laboratories, Derbyshire, UK, sponsored by The Lubrizol Corporation, September 28, 2004.

(7) Younger Laboratories, Inc. (1970) Sponsored by Monsanto, EPA/OTS #0545778

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-16174B

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06 JAN 19 AM 7:41

IUCLID Dataset

Existing Chemical	Substance ID: 104-76-7
CAS No.	104-76-7
EINECS Name	2-ethylhexan-1-ol
EINECS No.	203-234-3
Molecular Formula	C8H18O

Dataset created by: EUROPEAN COMMISSION - European Chemicals Bureau

This dossier is a compilation based on data reported by the European Chemicals Industry following 'Council Regulation (EEC) No. 793/93 on the Evaluation and Control of the Risks of Existing Substances'. All (non-confidential) information from the single datasets, submitted in the IUCLID/HEDSET format by individual companies, was integrated to create this document.

The data have not undergone any evaluation by the European Commission.

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European Chemicals Bureau

1.0.1 OECD and Company Information

Name: Alusuisse Italia Spa
Street: via del Pruneto, 40
Town: I-52027 S.Giovanni Valdarno (AR)
Country: Italy

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: Alusuisse Italia Spa
Street: via del Pruneto, 40
Town: I-52027 S.Giovanni Valdarno (AR)
Country: Italy
Phone: 055/940032
Telefax: 055/943936
Telex: 570447

Name: Atochem
Town: 92080 Paris la Defense
Country: France

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: Atochem
Street: 4, Cours Michelet
Town: 92080 Paris la Defense
Country: France

Name: BASF AG
Street: Karl-Bosch-Str
Town: 67056 Ludwigshafen
Country: Germany

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: BASF AG
Street: Karl-Bosch-Str
Town: 67056 Ludwigshafen
Country: Germany

Name: BASF Espanola S. A.
Town: 43080 Tarragona
Country: Spain

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: BASF Espanola S. A.
Town: 43080 Tarragona
Country: Spain

Name: BP Chemicals Ltd.
Street: Belgrave House, 76 Buckingham Palace Road
Town: SW1 WOSU London
Country: United Kingdom

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: BP Chemicals Ltd.
Street: 76, Buckingham Palace Road
Town: SW1 WOSU London
Country: United Kingdom

Name: BUNA GMBH
Street: Sparte Organica Bau G59
Town: 06258 Schkopau
Country: Germany

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: BUNA GMBH
Street: Sparte Organica Bau G59
Town: 06258 Schkopau
Country: Germany
Phone: 03461 49 2007
Telefax: 03461 49 2670

Name: Celanese GmbH
Street: Industriepark Höchst
Town: 65926 Frankfurt am Main
Country: Germany

Name: Ciba-Geigy SpA
Street: S.S.233 Km 20.5 Varesina
Town: I-21047 Saronno(VA)
Country: Italy
Phone: 39 2 96541
Telefax: 39 2 96701091

Name: CYTEC INDUSTRIES B.V.
Street: P.O.Box 5195 , Botlekweg 175
Town: 3197 ZH Rotterdam
Country: Netherlands

Name: ECEM European Chemical Marketing B.V.
Street: Hogehilweg 10
Town: 1101 CC Amsterdam
Country: Netherlands
Phone: 020-6912001
Telefax: 020-6911930

Name: Helm AG
Street: Nordkanalstrasse 28
Town: 20097 Hamburg
Country: Germany
Phone: +49402375-0
Telefax: +49402375-90
Telex: 2170150

Name: Hoechst AG
Town: 65903 Frankfurt/Main
Country: Germany

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: Hoechst AG
Street: Postfach 80 03 20 Brüningstrasse 50
Town: 65903 Frankfurt/Main
Country: Germany

Name: Huels AG
Street: Postfach
Town: 45764 Marl
Country: Germany

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: Huels AG
Street: Postfach
Town: D-45764 Marl
Country: Germany

Name: International Speciality Chemicals Ltd.
Street: Charleston Industries Estate, Hardley, Hythe
Town: SO45 32G Southampton
Country: United Kingdom

Name: Lubrizol Great Britain Limited
Street: P.O.Box 88
Town: DE56 1QN Belper, Derby
Country: United Kingdom
Phone: 332-842211
Telefax: 332-842303
Telex: 37445

Name: Neste Oxo AB
Town: 444 84 Stenungsund
Country: Sweden

Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Name: Neste Oxo AB
Town: 44484 Stenungsund
Country: Sweden
Phone: +46 303 85600
Telefax: +46 303 856 07
Telex: 27052 nestox S

Name: Petrasol B.V.
Street: P.O.Box 222
Town: 4200 AE Gorinchem
Country: Netherlands
Phone: +31 183 630555
Telefax: +31 183 632272
Telex: 23602 petr nl

Name: Vinyl Additives GmbH formerly CIBA Additive GmbH
Street: Chemiestrasse
Town: D-68623 Lampertheim
Country: Germany
Phone: +49(6206)15-0
Telefax: +49(6206)152511

Name: VOS B.V.
Street: Ondernemingsweg 1A
Town: 2404 HM Alphen aan den Rijn
Country: Netherlands
Phone: 31-172-431601
Telefax: 31-172-432494

1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

-

1.1 General Substance Information

Substance type: inorganic
Physical status: liquid

Substance type: organic
Physical status: liquid

Substance type:
Physical status:

1.1.1 Spectra

-

1.2 Synonyms

1-Ethyl-1-hexanol
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

1-Hexanol, 2-ethyl-
Source: Huels AG Marl

1-Hexanol, 2-ethyl- (8CI, 9CI)
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-EH
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethyl-1-hexanol
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-ethyl-1-hexanol
Remark: Also known as:
2-ethylhexyl alcohol
2-EH
Iso-octanol
Source: International Speciality Chemicals Ltd. Southampton

2-Ethylhexaan-1-ol
Source: VOS B.V. Alphen aan den Rijn

2-Ethylhexanol
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Huels AG Marl
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Vinyl Additives GmbH formerly CIBA Additive GmbH Lampertheim

2-Ethylhexanol iso-Octanol
Source: BUNA GMBH Schkopau
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BUNA GMBH Schkopau
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexanol-1
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BASF AG Ludwigshafen

BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexanol; 2-Ethylhexylalcohol; Isooctanol; Octylalcohol; 2-EH
Source: Atochem Paris la Defense
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexanol; ethylhexanol
Source: ISIS/RISKLINE release VI, 1997, Haskoning
Petrasol B.V. Gorinchem

2-Ethylhexyl alcohol
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexylalkohol
Source: Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Etil esanolo
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2EH
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

alcol 2-etilesilico
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Celanese GmbH Frankfurt am Main

Ethylhexanol
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Isooctanol
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Huels AG Marl
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

isoottanolo
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Octyl alcohol
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

Quantity 500 000 - 1 000 000 tonnes
Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Quantity more than 1 000 000 tonnes

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

Type: type
Category: Non dispersive use

Type: type
Category: Use in closed system

Type: type
Category: Wide dispersive use

Type: industrial
Category: Basic industry: basic chemicals

Type: industrial
Category: Chemical industry: used in synthesis

Type: industrial
Category: Paints, lacquers and varnishes industry

Type: industrial
Category: Polymers industry

Type: industrial
Category: Textile processing industry

Type: industrial
Category: other

Type: use
Category: Fuel additives
Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Type: use
Category: Fuel additives
Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Type: use
Category: Fuel additives

Type: use
Category: Intermediates

Type: use
Category: Lubricants and additives
Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Type: use
Category: Lubricants and additives
Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Type: use
Category: Lubricants and additives

Type: use
Category: Softeners
Source: ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Type: use
Category: Softeners

Type: use
Category: Solvents

Type: use
Category: other

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

Type of limit: MAK (DE)
Limit value:
Remark: Kein MAK-Wert festgelegt
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(1)

Type of limit: MAK (DE)
Limit value:
Country: Germany
Remark: MAK not established.
Source: Huels AG Marl

(2)

Type of limit: OES (UK)
Limit value: 271 mg/m3
Schedule: 8 hour(s)
Remark: UK OES not assigned specifically. Figure quoted is for Iso-octyl alcohol (mixed isomers) - from EH40 1998 edition.
Source: International Speciality Chemicals Ltd. Southampton

Type of limit: TLV (US)
Limit value: 250 mg/m3
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Type of limit:
Limit value:
Remark: No data on Occupational Exposure Limit Value.
Source: Atochem Paris la Defense

Type of limit:
Limit value:
Remark: No Occupational Exposure Limit available.
Source: Neste Oxo AB Stenungsund

1.9 Source of Exposure

Remark: PROFESSIONAL/OCCUPATIONAL EXPOSURE DURING PRODUCTION

Process description

1. Production of "oxo alcohols" (2-ethylhexanol, normal and iso-butanol) is performed through several steps of continuous and closed chemical processes.
The first step is the production of synthesis gas obtained by partial oxidation of natural gas.
This so called syngas is used to hydroformylate propylene, a reaction which produces a mixture of n- and isobutyraldehyde.

- 2-Ethylhexanol production
2ethylhexanol is produced by aldolisation of normal butyraldehyde, followed by hydrogenation and distillation.
- Storage and despatch of Oxo Alcohols
Oxo alcohols are stored in closed tanks where vent gas is collected and burnt in a residual gas incinerator.
There is no equipment opening during production, hence exposure to chemicals is quite limited.
Product despatch is done by road, rail, or ship mainly.

2. Number of sites
One production site located in Lavera, France.
3. Protective measures
Procedures and equipment used minimise personnel exposure. Workers and contractors wear gloves, safety glasses or goggies, and long sleeves clothes.
4. Industrial hygiene monitoring
Continuous on line explisimeters detect leaks.
Local explosivity analysis is made before maintenance work.
Outside operators are watching any abnormal noise or odor.
Routine analysis of hydrocarbon in atmosphere is done.
Worker have a yearly medical follow up.
COV monitoring program underway : will be finished in 18 months.

ENVIRONMENTAL EXPOSURE DURING PRODUCTION AND USE

1. Distribution pattern

Production lossed	ethyl-2-hexanol
to air	0.001 %
to water	0.004 %

2. Primary exposed environment
All spills are collected. Plant drainage is collected to chemical water sewer. This water is treated in a water treatment plant.

3. Release pattern
Point source and diffuse.

GENERAL USE PATTERN

100 % professional use.

ADDITIONAL INFORMATION

1. Indication of measured exposure levels.
Atmosphere analysis performed 2 times per year indicate an average value of 4 vpm of chemical expressed as CH4.
VOC monitoring program will allow a better follow up.

Source:
Atochem Paris la Defense
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Remark:
La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti.
Il processo dove viene impiegata la sostanza è di tipo discontinuo (per batch) e consiste essenzialmente nelle seguenti fasi:

- Reazione
- Purificazione
- Filtrazione

Tutte le fasi del processo vengono condotte a ciclo chiuso in quanto tutte le sostanze coinvolte nella sintesi chimica sono movimentate attraverso pompe , tubazioni, sistemi di trasferimento e apparecchiature di tipo chiuso.
Gli effluenti del processo sono i seguenti:
1) Acqua di reazione
2) Gas incondensabili

L'acqua di reazione, contenente tracce di sostanze organiche, viene raccolta e trasferita al trattamento di depurazione nell'impianto ecologico dello Stabilimento, quindi immessa n acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi immessi in atmosfera in conformità alle leggi nazionali vigenti (DPR 203/88).

Dati relativi alle emissioni

Acque trattate :

* tipo di emissione - puntiforme
* Durata emissione - continua

Emissioni atmosfera:

* tipo di emissione - puntiforme
* Portata - 25 Nm3/h per Ton. di sostanza
* durata emissione - continua

Fattori potenziali di esposizione umana

La sostanza ha un'alta temperatura di ebollizione ed una bassa tensione di vapore, presenta altresuna buona soglia olfattiva.Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.

Settori di impiego

La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

Country: Sweden

Remark: One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the production of plasticisers.

The production of 2-ethylhexanol is a closed process.

No 2-ethylhexanol is used in cosumer products.

Source: Neste Oxo AB Stenungsund

(3)

Remark: La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti.
Il processo dove viene impiegata la sostanza è di tipo discontinuo (per batch) e consiste essenzialmente nelle seguenti fasi:

- Reazione
- Purificazione
- Filtrazione

Tutte le fasi del processo vengono condotte a ciclo chiuso in quanto tutte le sostanze coinvolte nella sintesi chimica sono movimentate attraverso pompe , tubazioni, sistemi di trasferimento e apparecchiature di tipo chiuso.

Gli effluenti del processo sono i seguenti:
1) Acqua di reazione
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L'acqua di reazione, contenente tracce di sostanze organiche, viene raccolta e trasferita al trattamento di depurazione nell'impianto ecologico dello Stabilimento, quindi immessa n acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi immessi in atmosfera in conformità alle leggi nazionali vigenti (DPR 203/88).

Dati relativi alle emissioni

Acque trattate :

* tipo di emissione - puntiforme
* Durata emissione - continua

Emissioni atmosfera:

* tipo di emissione - puntiforme
* Portata - 25 Nm3/h per Ton. di sostanza
* durata emissione - continua

Fattori potenziali di esposizione umana

La sostanza ha un'alta temperatura di ebollizione ed una bassa tensione di vapore, presenta altresuna buona soglia olfattiva.Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.

Settori di impiego

La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Country: Sweden

Remark: One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the

production of plasticisers.

The production of 2-ethylhexanol is a closed process.

No 2-ethylhexanol is used in cosumer products.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(3)

Remark: La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti.
Il processo dove viene impiegata la sostanza è di tipo discontinuo (per batch) e consiste essenzialmente nelle seguenti fasi:

- Reazione
- Purificazione
- Filtrazione

Tutte le fasi del processo vengono condotte a ciclo chiuso in quanto tutte le sostanze coinvolte nella sintesi chimica sono movimentate attraverso pompe , tubazioni, sistemi di trasferimento e apparecchiature di tipo chiuso.
Gli effluenti del processo sono i seguenti:
1) Acqua di reazione
2) Gas incondensabili

L'acqua di reazione, contenente tracce di sostanze organiche, viene raccolta e trasferita al trattamento di depurazione nell'impianto ecologico dello Stabilimento, quindi immessa n acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi immessi in atmosfera in conformità alle leggi nazionali vigenti (DPR 203/88).

Dati relativi alle emissioni

Acque trattate :

* tipo di emissione - puntiforme
* Durata emissione - continua

Emissioni atmosfera:

* tipo di emissione - puntiforme
* Portata - 25 Nm3/h per Ton. di sostanza
* durata emissione - continua

Fattori potenziali di esposizione umana
La sostanza ha un'alta temperatura di ebollizione ed una

bassa tensione di vapore, presenta altresuna buona soglia olfattiva.Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.

Settori di impiego

La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Country: Sweden

Remark: One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the production of plasticisers.

The production of 2-ethylhexanol is a closed process.

No 2-ethylhexanol is used in cosumer products.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(3)

1.10.1 Recommendations/Precautionary Measures

-

1.10.2 Emergency Measures

-

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

Classified by: KBwS (DE)
Labelled by: KBwS (DE)
Class of danger: 2 (water polluting)
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

Classified by: KBwS (DE)
Labelled by:
Class of danger: 2 (water polluting)
Country: Germany
Remark: Kenn-Nr. 134
Source: Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(4)

Classified by: KBwS (DE)
Labelled by: KBwS (DE)
Class of danger: 2 (water polluting)
Country: Germany
Remark: Katalognummer 134
Source: Huels AG Marl

(2)

1.14.2 Major Accident Hazards

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

(5)

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Source: Hoechst AG Frankfurt/Main

(6)

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Country: Germany
Remark: Stoerfallverordnung 1991
Source: Huels AG Marl

(2)

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(6)

1.14.3 Air Pollution

Classified by: TA-Luft (DE)
Labelled by: TA-Luft (DE)
Number: 3.1.7 (organic substances)
Class of danger: III
Source: BASF Espanola S. A. Tarragona

(7)

Classified by: TA-Luft (DE)
Labelled by:
Number: 3.1.7 (organic substances)
Class of danger: III
Remark: Selbsteinstufung
Source: Hoechst AG Frankfurt/Main

(8)

Classified by: TA-Luft (DE)
Labelled by: TA-Luft (DE)
Number: 3.1.7 (organic substances)
Class of danger: III
Country: Germany
Remark: Appendix E
Source: Huels AG Marl

(2)

Classified by: TA-Luft (DE)
Labelled by:
Number: 3.1.7 (organic substances)
Class of danger: III
Remark: Selbsteinstufung
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

1.15 Additional Remarks

Remark: Possibilità di eliminazione

La sostanza ha una bassa solubilità in acqua (ca 0.1 mg/l); può essere eliminata per ossidazione biologica in appositi impianti di trattamento.
La sostanza può essere eliminata anche per ossidazione termica in appositi impianti di incenerimento con recupero energetico e controllo emissioni all'atmosfera secondo la normativa vigente.

Informazioni relative al trasporto

La sostanza che viene importata ed utilizzata come materia prima viaggia su carri cisterna ferroviari secondo la normativa Internazionale RID appartenendo alla classe 3 ordinale 32° c), indice KEMLER e n° ONU 30/1987.

Tipo del numero: ferrocisterna per prodotti RID

Quantità media
trasportata : 56.000 kg

Ferrocisterne/mese: 4

Misure di controllo
durante il trasporto: Il prodotto viaggia con la documentazione stabilita dalle leggi vigenti in materia (normativa RID)

Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Remark: Wasserschadstoffklasse 2
Source: BUNA GMBH Schkopau

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2.1 Melting Point

Value: -76 - 70 degree C
Source: Neste Oxo AB Stenungsund
(10)

Value: -76 - 70 degree C
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
(11)

Value: -76 - 70 degree C
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(11)

Value: < -60 degree C
Method: other: DIN 3016
Source: Neste Oxo AB Stenungsund
(12)

Value: < -60 degree C
Method: other: DIN 3016
Source: Hoechst AG Frankfurt/Main
(8)

Value: < -60 degree C
Method: other: DIN 3016
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

2.2 Boiling Point

Value: 183.5 - 185 degree C at 1013 hPa
GLP: no
Source: Neste Oxo AB Stenungsund
(13)

Value: 183.5 - 185 degree C at 1013 hPa
GLP: no
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
(11)

Value: 183.5 - 185 degree C at 1013 hPa
GLP: no
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(11)

Value: = 184 degree C
Method: other: DIN 53 171
Source: Neste Oxo AB Stenungsund
BASF AG Ludwigshafen
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(14)

Value: = 184.3 degree C at 1013 hPa
Source: ECEM European Chemical Marketing B.V. Amsterdam

Value: 184.5 degree C at 1013 hPa
Source: Neste Oxo AB Stenungsund
(15)

Value: = 184.5 degree C at 1013 hPa
Source: Hoechst AG Frankfurt/Main
(8)

Value: = 184.5 degree C at 1013 hPa
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

2.3 Density

Type: density
Value: = .83 g/cm3 at 20 degree C
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(11)

Type:
Value: ca. .832 - .833 at 20 degree C
Source: ECEM European Chemical Marketing B.V. Amsterdam

Type: density
Value: = .832 g/cm3 at 20 degree C
Method: other: DIN 51757
Source: Neste Oxo AB Stenungsund
(15)

Type: density
Value: = .832 g/cm3 at 20 degree C
Method: other: DIN 51757
Source: Hoechst AG Frankfurt/Main
(8)

Type: density
Value: = .832 g/cm3 at 20 degree C
Method: other: DIN 51757
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

Type: density
Value: = .84 g/cm3 at 20 degree C
Source: BASF AG Ludwigshafen
(16)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: = .05 at 20 degree C
Source: ECEM European Chemical Marketing B.V. Amsterdam

Value: .144 hPa at 20 degree C
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(14)

Value: = .144 hPa at 20 degree C
Source: BASF AG Ludwigshafen
(14)

Value: .4 hPa at 20 degree C
Method: other (calculated): calculated
Source: Neste Oxo AB Stenungsund
(15)

Value: = .4 hPa at 20 degree C
Method: other (calculated)
Source: Hoechst AG Frankfurt/Main
(8)

Value: = .4 hPa at 20 degree C
Method: other (calculated)
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

Value: ca. .13 hPa at 25 degree C
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(17)

Value: 2.9 hPa at 50 degree C
Method: other (calculated): calculated
Source: Neste Oxo AB Stenungsund
(15)

Value: = 2.9 hPa at 50 degree C
Method: other (calculated)
Source: Hoechst AG Frankfurt/Main
(8)

Value: = 2.9 hPa at 50 degree C
Method: other (calculated)
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

2.5 Partition Coefficient

log Pow: = 2.28
Method: other (calculated): calculated; Leo and Hansch
Year:
Source: Neste Oxo AB Stenungsund
(15)

log Pow: = 2.28
Method: other (calculated): Leo und Hansch
Year:
Source: Hoechst AG Frankfurt/Main
(8)

log Pow: = 2.28
Method: other (calculated): Leo und Hansch
Year:
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

log Pow: 2.809
Method: other (calculated)
Year:
Remark: Calculated according to Leo and Hansch, MedChem-Programm, Version 1989 (POMONA89)
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

log Pow: ca. 3
Method:
Year:
Source: BASF AG Ludwigshafen
(18)

log Pow: = 3.1
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year: 1981
GLP: no data
Source: Neste Oxo AB Stenungsund
(19)

log Pow: = 3.1
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year: 1981
GLP: no data
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
(20)

log Pow: = 3.1
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year: 1981
GLP: no data
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(20)

2.6.1 Water Solubility

Value: = .1 at 20 degree C
Source: ECEM European Chemical Marketing B.V. Amsterdam

Value: ca. 1 g/l at 20 degree C
Source: Neste Oxo AB Stenungsund
(16)

Value: = 1 g/l at 20 degree C
pH: = 7 at 1 g/l and 20 degree C
Source: Neste Oxo AB Stenungsund
(15)

Value: ca. 1 g/l at 20 degree C
Source: BASF AG Ludwigshafen
(14)

Value: = 1 g/l at 20 degree C
pH: = 7 at 1 g/l and 20 degree C
Source: Hoechst AG Frankfurt/Main
(8)

Value: ca. 1 g/l at 20 degree C
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
(14)

Value: = 1 g/l at 20 degree C
pH: = 7 at 1 g/l and 20 degree C
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

Value: ca. 1 g/l at 20 degree C
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(14)

Value: = 1100 mg/l at 25 degree C
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(21)

2.6.2 Surface Tension

-

2.7 Flash Point

Value: = 73 degree C
Type: closed cup
Method:
Year:
Source: ECEM European Chemical Marketing B.V. Amsterdam

Value: = 75 degree C
Type:
Method: other: DIN 51758
Year:
Source: Neste Oxo AB Stenungsund
(15)

Value: = 75 degree C
Type:
Method: other: DIN EN 22719, ISO 2719
Year:
Source: Hoechst AG Frankfurt/Main
(8)

Value: = 75 degree C
Type:
Method: other: DIN EN 22719, ISO 2719
Year:
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

Value: = 76 degree C
Type:
Method: other: DIN 51 758
Year:
Source: Neste Oxo AB Stenungsund
BASF AG Ludwigshafen
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(14)

Value: = 82 degree C
Type: closed cup
Method: other
Year:
Remark: Method: DIN 51758
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Celanese GmbH Frankfurt am Main

(22)

2.8 Auto Flammability

Value: = 270 degree C
Method: other: DIN 51 794
Source: Neste Oxo AB Stenungsund
BASF AG Ludwigshafen
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(14)

Value: = 305 degree C
Method: other: DIN 51794
Remark: Auto-ignition temperature
Source: Neste Oxo AB Stenungsund

(15)

Value: = 305 degree C
Method: other: DIN 51794
Remark: Zuendtemperatur
Source: Hoechst AG Frankfurt/Main

(8)

Value: = 305 degree C
Method: other: DIN 51794
Remark: Zuendtemperatur
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value: 330 degree C
Method: other
Remark: Method: DIN 51794
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(20)

2.9 Flammability

Result: other: when heated vapors may form explosive mixtures with air
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2.10 Explosive Properties

Result: other
Remark: Explosionsgrenze: 1.1 - 12.7 Vol.-%
Source: Hoechst AG Frankfurt/Main
(8)

Result: other
Remark: Explosionsgrenze: 1.1 - 12.7 Vol.-%
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

Result: other: Explosionsgrenzen 1.1 - 7.4 Vol.%
Source: BASF AG Ludwigshafen
(16)

Result:
Remark: Explosive limits in air: 1.1 -12.7 vol-%
Source: Neste Oxo AB Stenungsund
(15)

2.11 Oxidizing Properties

Result:
Source: Neste Oxo AB Stenungsund

2.12 Additional Remarks

Remark: Remark 1: Viscosity
12 mm2/s at 20 degrees C
35 mm2/s at 0 degrees C
Remark 2: Henry's law constant: 2.65 E-5 atm x m3 x mole-1
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(23) (24)

Remark: Dynamic viscosity: 10 mPas at 20 degrees C.

(Method: DIN 51562)
Source: Neste Oxo AB Stenungsund
(15)

Remark: Viskositaet: 8.8 mPa.s (20 Grad C)
Source: BASF AG Ludwigshafen
(16)

Remark: Dynamische Viskositaet bei 20 Grad C: 10 mPas
(Methode: DIN 51562)
Source: Hoechst AG Frankfurt/Main
(8)

Remark: Dynamische Viskositaet bei 20 Grad C: 10 mPas
(Methode: DIN 51562)
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

Remark: Gefährliche Reaktionen: mit Oxidationsmitteln
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001296 cm3/(molecule * sec)
Degradation: ca. 50 % after 9.9 hour(s)
Method: other (calculated): calculated; AOPWIN, Version 1.55, April 1994, Syracuse Research
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: No study located.
Source: Neste Oxo AB Stenungsund

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001296 cm3/(molecule * sec)
Degradation: ca. 50 % after 9.9 hour(s)
Method: other (calculated): AOPWIN, Version 1.55, April 1994, Syracuse Research
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(25)

3.1.2 Stability in Water

Type:
Method:
Year: **GLP:**
Test substance:
Remark: Study not located.
Source: Neste Oxo AB Stenungsund

3.1.3 Stability in Soil

Type: **Radiolabel:**
Concentration:
Cation exch. capac.
Microbial biomass:
Method:
Year: **GLP:**
Test substance:
Remark: Koc = 105 (calculated by equation 4-5 in Lyman, et al (1981).
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(26)

3.2 Monitoring Data (Environment)

Type of measurement: background concentration
Medium: surface water
Result: 66-111 ug/l in Hayashida river, Japan.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(27)

Type of measurement: background concentration
Medium: surface water
Result: 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source: Neste Oxo AB Stenungsund

(28)

Type of measurement: background concentration
Medium: surface water
Remark: 2-Ethylhexanol detected in Mersey estaury 1990.
Source: Neste Oxo AB Stenungsund

(29)

Type of measurement: background concentration
Medium: drinking water
Remark: 2-Ethylhexanol detected in "tap water", Japan 1980.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(30)

Type of measurement: background concentration
Medium: surface water
Result: 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(28)

Type of measurement: background concentration
Medium: surface water
Remark: 2-Ethylhexanol detected in Mersey estaury 1990.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(29)

Type of measurement: background concentration
Medium: surface water
Result: 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(28)

Type of measurement: background concentration
Medium: surface water
Remark: 2-Ethylhexanol detected in Mersey estaury 1990.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(29)

Type of measurement:
Medium: surface water
Result: Saskatchewan River, 8 and 20 km downstream from Nipawin, 2-ethylhexanol detected, not quantified.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(31)

Type of measurement:
Medium: surface water
Result: West Valley, New York: 3.6-8.1 mg/l
Source: Neste Oxo AB Stenungsund

(32)

Type of measurement:
Medium: surface water
Result: West Valley, New York: 3.6-8.1 mg/l
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(32)

Type of measurement:
Medium: surface water
Result: West Valley, New York: 3.6-8.1 mg/l
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(32)

3.3.1 Transport between Environmental Compartments

Type:
Media:
Method:
Year:
Remark: No study located.
Source: Neste Oxo AB Stenungsund

3.3.2 Distribution

Media: other
Method: Calculation according Mackay, Level I
Year:
Remark: Media: air-water-sediment-soil.

Result: air 16%, water 53%, sediment 25%, soil 5.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(33)

3.4 Mode of Degradation in Actual Use

Remark: Biological degradation is expected to be the main mode of degradation.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 3.16 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: = 55 % after 17 day
Method: Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(34)

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 6.32 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: = 68 % after 17 day
Method: Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source: Neste Oxo AB Stenungsund

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 6.32 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: = 68 % after 17 day
Method: Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(34)

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 6.32 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: = 68 % after 17 day
Method: Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(34)

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 250 mg/l
Degradation: = 100 % after 5 day
Result: inherently biodegradable
Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1985 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(35)

Type: aerobic
Inoculum: activated sludge, industrial, non-adapted
Degradation: > 95 % after 5 day
Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1980 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: Non-biological elimination: 20-30%
Source: Neste Oxo AB Stenungsund

(36)

Type: aerobic
Inoculum: activated sludge, industrial, non-adapted
Degradation: > 95 % after 5 day
Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1980 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: Eliminierung durch nicht biol. Vorgänge 20 - 30 %
Source: Hoechst AG Frankfurt/Main

(37)

Type: aerobic
Inoculum: activated sludge, industrial, non-adapted
Degradation: > 95 % after 5 day
Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1980 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: Eliminierung durch nicht biol. Vorgänge 20 - 30 %
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(37)

Type: aerobic
Inoculum: activated sludge, industrial, non-adapted
Concentration: 249 mg/l related to Test substance
Degradation: = 97 % after 7 day
Kinetic:
1 day = 23 %
2 day = 36 %
5 day = 96 %
7 day = 97 %
Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund

Type: aerobic
Inoculum: activated sludge, industrial, non-adapted
Concentration: 249 mg/l related to Test substance
Degradation: = 97 % after 7 day
Kinetic:
1 day = 23 %
2 day = 36 %
5 day = 96 %
7 day = 97 %
Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Hoechst AG Frankfurt/Main

(38)

Type: aerobic
Inoculum: activated sludge, industrial, non-adapted
Concentration: 249 mg/l related to Test substance
Degradation: = 97 % after 7 day
Kinetic:
1 day = 23 %
2 day = 36 %
5 day = 96 %
7 day = 97 %
Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(38)

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 83 mg/l related to Test substance
Degradation: = 88 % after 17 day
Method: other: EEC Directive 79-831 Annex V Part C
Year: 1984 **GLP:**
Test substance:
Remark: Degradation is the measured BOD as percent of ThOD.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(39)

Type: aerobic
Inoculum: other: Belebtschlamm einer kommunalen Klaeranlage
Concentration: 83 mg/l related to Test substance
Degradation: = 88 % after 17 day
Method: other: EEC Directive 79-831 Annex V Part C: Methods for the determination of ecotoxicity. Degradation - Biotic Degradation. Manometric Respirometry
Year: 1984 **GLP:**
Test substance:
Remark: Der Abbauwert ist der gemessene biochemische Sauerstoffbedarf BSB als Prozentwert des theoretischen Sauerstoffbedarfs (ThSB).
Source: BASF AG Ludwigshafen

(40)

Type: aerobic
Inoculum: activated sludge, non-adapted
Method:
Year: **GLP:**
Test substance:
Remark: Method: BOD5-20 fresh and sea water.

Results:	Fresh water	Sea water
	BOD5=26%	BOD5=58%
	BOD10=75%	BOD10=64%
	BOD15=78%	BOD15=84%
	BOD20=86%	BOD20=100%

Source: Neste Oxo AB Stenungsund

(41)

Type: aerobic
Inoculum: activated sludge, non-adapted
Method:
Year: **GLP:**
Test substance:
Remark: Method: BOD5-20 fresh and sea water.

Results:	Fresh water	Sea water
	BOD5=26%	BOD5=58%
	BOD10=75%	BOD10=64%
	BOD15=78%	BOD15=84%
	BOD20=86%	BOD20=100%

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(42)

Type: aerobic
Inoculum: activated sludge, non-adapted
Method:
Year: **GLP:**
Test substance:
Remark: Method: BOD5-20 fresh and sea water.

Results:	Fresh water	Sea water
	BOD5=26%	BOD5=58%
	BOD10=75%	BOD10=64%
	BOD15=78%	BOD15=84%
	BOD20=86%	BOD20=100%

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(42)

Type: aerobic
Inoculum: aerobic microorganisms
Concentration: .1 mg/l
Method:
Year: **GLP:**
Test substance:
Remark: Test medium: pure bacteria culture suspension isolated from activated sludge.

Results: Normal sewage (domestic waste water)
0% degraded after 24 h.
100% degraded after 5.6 days.

Adapted sewage (industrial effluent)
100% degraded after 24h.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(43)

Type: aerobic
Inoculum:
Method:
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund

(44)

Type: aerobic
Inoculum:
Method:
Year: **GLP:**
Test substance:
Result: Method: Secondary effluent from municipal and industrial waste water treatment plants was used as seed (25-55 ml/l).

Results:	Municipal	Industrial
BOD5/COD	0.70	0.60
BOD10/COD	0.81	0.77
BOD20/COD	0.87	0.86

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Type: aerobic
Inoculum:
Method:
Year: **GLP:**
Test substance:
Result: Method: Secondary effluent from municipal and industrial waste water treatment plants was used as seed (25-55 ml/l).

Results:	Municipal	Industrial
BOD5/COD	0.70	0.60
BOD10/COD	0.81	0.77
BOD20/COD	0.87	0.86

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

3.6 BOD5, COD or BOD5/COD Ratio

-

3.7 Bioaccumulation

Species:
Exposure period:
Concentration:
BCF: ca. 27
Elimination:
Method: other: Calcualtion based on water solubility
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund

(45)

Species:
Exposure period:
Concentration:
BCF: ca. 27
Elimination:
Method: other: Calcualtion based on water solubility
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(46)

Species:
Exposure period:
Concentration:
BCF: ca. 27
Elimination:
Method: other: Calcualtion based on water solubility
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(46)

3.8 Additional Remarks

-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 43 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: 96 - 144
Method: other: diatary exposure
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Result: No effect on mortality
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(47)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: 27 - 29.5
Method: other: in Anlehnung an EPA-Guideline
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(48)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
NOEC: = 10
LC50: 29.7
Method: other: keine Angaben
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(46)

Type: other
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 5 day
Unit: mg/l **Analytical monitoring:** no data
LC50: = 24
Method: other: keine Angaben
Year: **GLP:** no data
Test substance: no data
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test condition: Species: fry, 0.15 g

Test condition: 15 degrees C, pH=7

(49)

Type: other
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: > 7.5
Method: other: keine Angaben
Year: **GLP:** no data
Test substance: no data
Remark: Fry, 0.15 g
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test condition: 20 degrees C; pH = 7

(49)

Type: flow through
Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 43 hour(s)
Unit: mg/l **Analytical monitoring:**
LC0: 96 - 144
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Method: diatary exposure.

Result: No effect on mortality.
Source: Neste Oxo AB Stenungsund

(47)

Type: flow through
Species: Leuciscus idus melanotus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
NOEC: = 14
LC50: = 17.1
LC100: = 21
Method: Directive 84/449/EEC, C.1 "Acute toxicity for fish"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(50)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:**
LC50: 27 - 29.5
Method: other
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund

(48)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:**
NOEC: = 10
LC50: 29.7
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund

(46)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: 32 - 37
Method: other: Range finding acute toxicity test.
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(51)

Type: other
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 5 day
Unit: mg/l **Analytical monitoring:**
LC50: = 24
Method:
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund
Test condition: Species: fry, 0.15 g

Test condition: 15 degrees C, pH=7

(52)

Type: other
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:**
LC50: > 7.5
Method:
Year: **GLP:**
Test substance:
Remark: Fry, 0.15 g
Source: Neste Oxo AB Stenungsund
Test condition: 20 degrees C; pH = 7

(49)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: 39
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(20)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: 39
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(20)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: = 44
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(46)

Species: Artemia salina (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: = 19
Method: other: keine Angaben
Year: **GLP:** no data
Test substance: no data
Remark: Species: seawater
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(42)

Species: Artemia salina (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:**
EC50: = 19
Method:
Year: **GLP:**
Test substance:
Remark: Species: seawater
Source: Neste Oxo AB Stenungsund
(42)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: 39
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
(53)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:**
EC50: = 44
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
(54)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 26
Method: other: Screening test
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(55)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Chlorella emersonii (Algae)
Endpoint: growth rate
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
NOEC: = 10
EC50: 10 - 50
Method: other: keine Angaben
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Method: 22 degrees C, air was passed through the culture.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(49)

Species: Chlorella emersonii (Algae)
Endpoint: growth rate
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
NOEC: = 10
EC50: 10 - 50
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Method: 22 degrees C, air was passed through the culture.
Source: Neste Oxo AB Stenungsund

(56)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** yes
NOEC: =
EC10: = 3.2
EC50: = 11.5
EC90 : ca. 41.1
Method: Directive 87/302/EEC, part C, p. 89 "Algal inhibition test"
Year: 1988 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(57)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC10: = 1.3
EC50: = 13.3
EC90 : = 138.5
Method: other: Algal growth inhibition test, UBA
Year: 1984 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(58)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 18 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC10: = 540
Method: other: DIN 38412 Part 8
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(20)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 18 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC10: = 540
Method: other: DIN 38412 Part 8
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(20)

Type: aquatic
Species: activated sludge, domestic
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
SG : ca. 300
Method: ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
Year: 1980 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: SG = Schädlichkeitsgrenze
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(37)

Type: aquatic
Species: activated sludge, domestic
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:**
SG : ca. 300
Method: ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
Year: 1980 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: SG= Schädlichkeitgrenze
Source: Neste Oxo AB Stenungsund

(36)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 18 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC10: = 540
Method: other: DIN 38412 Part 8
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund

(59)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species:
Endpoint:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Study not located.
Source: Neste Oxo AB Stenungsund

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species:
Endpoint:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Study not located.
Source: Neste Oxo AB Stenungsund

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:
Species:
Endpoint:
Exposure period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: No study located.
Source: Neste Oxo AB Stenungsund

4.6.2 Toxicity to Terrestrial Plants

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: Study not located.
Source: Neste Oxo AB Stenungsund

4.6.3 Toxicity to other Non–Mamm. Terrestrial Species

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: No study located.
Source: Neste Oxo AB Stenungsund

4.7 Biological Effects Monitoring

Remark: Study not located.
Source: Neste Oxo AB Stenungsund

4.8 Biotransformation and Kinetics

Type:
Remark: Study not located.
Source: Neste Oxo AB Stenungsund

4.9 Additional Remarks

-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 3730 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: 99.5%
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(60)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 1516 - 2774 mg/kg bw
Method:
Year: **GLP:**
Test substance: no data
Source: Neste Oxo AB Stenungsund

(61)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 3870 - 5520 mg/kg bw
Method:
Year: **GLP:**
Test substance: other TS: technical grade
Remark: 2-Ethylhexanol (technical grade) was administered to a total of 70 female rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Celanese GmbH Frankfurt am Main

(62)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 3700
Method:
Year: **GLP:** no
Test substance: no data
Remark: Range of values: 3.61-5.52 ml/kg (3.0-4.6 g/kg)
2-Ethylhexanol was given undiluted; no further details reported.
Source: Neste Oxo AB Stenungsund

(63)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 7000 mg/kg bw
Method:
Year: **GLP:** no
Test substance: no data
Remark: Result: 49 male albino rats (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 5, 6, 8, 10, 12, and 15 g/kg bw. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(64)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 1516 - 2774 mg/kg bw
Method:
Year: **GLP:**
Test substance: no data
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(65)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 3700
Method:
Year: **GLP:** no
Test substance: no data
Remark: Range of values: 3.61-5.52 ml/kg (3.0-4.6 g/kg)
2-Ethylhexanol was given undiluted; no further details reported.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(66)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 1516 - 2774 mg/kg bw
Method:
Year: **GLP:**
Test substance: no data
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(65)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 3700
Method:
Year: **GLP:** no
Test substance: no data
Remark: Range of values: 3.61-5.52 ml/kg (3.0-4.6 g/kg)
2-Ethylhexanol was given undiluted; no further details reported.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(66)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: = 3768 mg/kg bw
Method:
Year: **GLP:**
Test substance: no data
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(67)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: 3280 - 4460 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: technical grade
Remark: Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice.
Source: Neste Oxo AB Stenungsund

(68)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: 2870 - 3610 mg/kg bw
Method:
Year: **GLP:**
Test substance: other TS: 2-EH technical grade
Remark: Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 femal mice.
Source: Neste Oxo AB Stenungsund

(69)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: = 3580 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Remark: Range of values: 2900-4420 mg/kg

2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and adminisered to a total of 70 male mice. The LD50 was calculated 2 days after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(62)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: = 2500 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Remark: Range of values: 2090-3010 mg/kg.
2-Ethylhexanol (technical grade, undiluted) was administered to a total of 70 female mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund

Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(62)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: 3280 - 4460 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: technical grade
Remark: Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(62)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: 2870 - 3610 mg/kg bw
Method:
Year: **GLP:**
Test substance: other TS: 2-EH technical grade
Remark: Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 femal mice.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(62)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: 3280 - 4460 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: technical grade
Remark: Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(62)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: 2870 - 3610 mg/kg bw
Method:
Year: **GLP:**
Test substance: other TS: 2-EH technical grade
Remark: Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 femal mice.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(62)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 1470 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund

(70)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 1180 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Remark: 2-Ethylhexanol (technical grade, undiluted) was administered to a total of 12 male rabbits. The LD50 was calcualted 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(62)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 1470 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(66)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 1470 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(66)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: = 600 mg/kg bw
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source: Neste Oxo AB Stenungsund

(71)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: 1220 - 2820 mg/kg bw
Method:
Year: **GLP:**
Test substance: other TS: 2-EH technical grade
Remark: 2-Ethylhexanol (technical grade) was administered to a total of 12 male guinea pigs. The LD50 was calculated 1 day after the test substance administration.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(62)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: = 600 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Remark: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source: Neste Oxo AB Stenungsund

(72)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: = 600 mg/kg bw
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source: Neste Oxo AB Stenungsund

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(64)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: = 600 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Remark: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(64)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: = 600 mg/kg bw
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(64)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: = 600 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Remark: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(64)

5.1.2 Acute Inhalation Toxicity

Type: other
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 4 hour(s)
Value:
Method:
Year: **GLP:**
Test substance:
Remark: Result: 2 groups of 6 Sprague-Dawley rats (3 male, 3 female) were exposed once to a vapor concentration of 0.89 mg/l and an aerosol/vapor concentration of 5.3 mg/l. Exposure was for 4 hrs, followed by a 7-day observation period. All animals exposed to to 5.3 mg/l died within 48 hrs of exposure, while animals of the other exposure group survived.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(73)

Type: other
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: 99.5%
Remark: Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motilty, slight to moderate dyspnoea, and moderate irritation of the eyes, nose , pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.
Source: Neste Oxo AB Stenungsund

(74)

Type: other
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: 99.5%
Remark: Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motilty, slight to moderate dyspnoea, and moderate irritation of the eyes, nose , pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(60)

Type: other
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: 99.5%
Remark: Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motilty, slight to moderate dyspnoea, and moderate irritation of the eyes, nose , pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(60)

Type: other
Species: mouse
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value: 44 ppm
Method:
Year: **GLP:**
Test substance:
Remark: Result: 44 ppm 2-ethylhexanol caused a 50% reduction in respiratory frequency in mice.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(75)

Type: other
Species: mouse
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: purity 99.5%
Remark: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.
Source: Neste Oxo AB Stenungsund

(76)

Type: other
Species: mouse
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: purity 99.5%
Remark: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(60)

Type: other
Species: mouse
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: purity 99.5%
Remark: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic

toxicity were not pronounced and consisted primarily of central nervous system depression.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(60)

Type: other: Dampfinhalation
Species: mouse
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value:
Method: other: interne Richtlinie der Hoechst AG
Year: 1951 **GLP:** no
Test substance: other TS
Remark: 2 ml Substanz in 7 Liter Luftraum verdampft rufen keine Letalität hervor.
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test substance: Substanzreinheit > 98 %

(77)

Type: other: Vapor inhalation
Species: mouse
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value:
Method: other: guidelines of Hoechst AG
Year: 1951 **GLP:** no
Test substance: other TS
Remark: 2 ml of 2-Ethylhexanol (vapour) in 7 l of air resulted in no lethal effects.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test substance: 2-Ethylhexanol concentration: > 98%

(77)

Type: other
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: purity 99.5%
Remark: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.
Source: Neste Oxo AB Stenungsund

(76)

Type: other
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: purity 99.5%
Remark: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(60)

Type: other
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value:
Method:
Year: **GLP:** no
Test substance: other TS: purity 99.5%
Remark: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic

toxicity were not pronounced and consisted primarily of central nervous system depression.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(60)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 3000 mg/kg bw
Method: OECD Guide-line 402 "Acute dermal Toxicity"
Year: 1981 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(78)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 1980 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Source: Neste Oxo AB Stenungsund

(79)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: > 2600 mg/kg bw
Method:
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: 2-ethylhexanol did not produce any clinical signs of toxicity.
Source: Neste Oxo AB Stenungsund

(76)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 1980 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(65)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: > 2600 mg/kg bw
Method:
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: 2-ethylhexanol did not produce any clinical signs of toxicity.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(60)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 1980 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(65)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: > 2600 mg/kg bw
Method:
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: 2-ethylhexanol did not produce any clinical signs of toxicity.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(60)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 937 mg/kg bw
Method:
Year: **GLP:**
Test substance: other TS: 2-EH technical grade
Remark: Range of values: 860-1020 mg/kg.
2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund

(80)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: 568 - 739 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: 2-EH technical grade
Remark: Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal rats.The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(81)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 650 mg/kg bw
Method:
Year: **GLP:** no
Test substance:
Remark: Rats promtly developed an irregular gait, dragging of hind legs, breathing became gasping, even on lower doses; rats were sound asleep in 10 min.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(82)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 937 mg/kg bw
Method:
Year: **GLP:**
Test substance: other TS: 2-EH technical grade
Remark: Range of values: 860-1020 mg/kg.
2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(81)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 937 mg/kg bw
Method:
Year: **GLP:**
Test substance: other TS: 2-EH technical grade
Remark: Range of values: 860-1020 mg/kg.
2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(81)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: 845 - 939 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: 2-EH technical grade
Remark: Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 70 male mice.The LD50 was calculated 1 day after the administration of the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(81)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: 726 - 801 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: 2-EH technical grade
Remark: Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund

(83)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: 726 - 801 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: 2-EH technical grade
Remark: Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(81)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: 726 - 801 mg/kg bw
Method:
Year: **GLP:** no
Test substance: other TS: 2-EH technical grade
Remark: Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(81)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: s.c.
Value:
Method:
Year: **GLP:** no
Test substance:
Remark: Range of values: 6.67-13.0 ml/kg (5.54-10.79 g/kg).
2-Ethylhexanol was given to female rats; no further details given.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(66)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1981 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: Method :2-Ethylhexanol was applied under occlusion to the skin of 3 male rabbits for 4 hours.

Result: An irritation index of 6.75/8 was determined.
redness: x=3.33
edema : x=4.00
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Celanese GmbH Frankfurt am Main

(84)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: moderately irritating
EC classificat.:
Method:
Year: **GLP:** no
Test substance:
Remark: Method: Single dermal application, shaved dorsal skin, 24 hr occlusion.

Result: moderate irritation
(scale:slight-moderate-marked-severe)
Not classifiable according to current EEC directives.
Source: Neste Oxo AB Stenungsund

(76)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result:
EC classificat.:
Method:
Year: **GLP:** no
Test substance:
Remark: Irritation Index: 3/10.
Not classifiable according to current EEC directives.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(65)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: highly irritating
EC classificat.:
Method: other: guidelines of Hoechst AG
Year: 1978 **GLP:** no
Test substance: no data
Remark: 0.5 ml of 2-Ethylhexanol was applied under occlusion on unabraded skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.
Source: Neste Oxo AB Stenungsund

(85)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.: irritating
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: BASF AG Ludwigshafen

(86)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: highly irritating
EC classificat.:
Method: other: interne Richtlinie der Hoechst AG
Year: 1978 **GLP:** no
Test substance: no data
Remark: 0.5 ml okklusiv auf die unverletzte Haut, Einwirkzeit 1, 2, 4 und 24 Stunden.
nicht einstufbar, Reizerscheinungen nach 7 Tagen nicht reversibel.
Source: Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(87)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: moderately irritating
EC classificat.:
Method:
Year: **GLP:** no
Test substance:
Remark: Method: Single dermal application, shaved dorsal skin, 24 hr occlusion.

Result: moderate irritation
(scale:slight-moderate-marked-severe)
Not classifiable according to current EEC directives.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(60)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: highly irritating
EC classificat.:
Method: other: guidelines of Hoechst AG
Year: 1978 **GLP:** no
Test substance: no data
Remark: 0.5 ml of 2-Ethylhexanol was applied under occlusion on unabraded skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(87)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: moderately irritating
EC classificat.:
Method:
Year: **GLP:** no
Test substance:
Remark: Method: Single dermal application, shaved dorsal skin, 24 hr occlusion.

Result: moderate irritation
(scale:slight-moderate-marked-severe)
Not classifiable according to current EEC directives.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(60)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: highly irritating
EC classificat.:
Method: other: guidelines of Hoechst AG
Year: 1978 **GLP:** no
Test substance: no data
Remark: 0.5 ml of 2-Ethylhexanol was applied under occlusion on unabraded skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(87)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method: Draize Test
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: 2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72 hrs), 0 (7 days).
Not classifiable according to current EEC directives.
Source: Neste Oxo AB Stenungsund

(88)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1981 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: Irritation Index: 28.6/110
cornea: x=1.44
iris: x=0.89
conjunctiva: redness: x=2.56
chemosis:x=0.78
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(89)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method:
Year: **GLP:** no
Test substance:
Remark: Instillation into the conjunctival sac of 20 ug caused moderately severe irritation of the cornea.
Not classifiable according to current EEC directives.
Source: Neste Oxo AB Stenungsund

(90)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method:
Year: **GLP:** no data
Test substance: no data
Remark: The test substance was reported to be irritating to rabbit eyes; no details reported.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(91)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method: Draize Test
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: 2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72 hrs), 0 (7 days).

Not classifiable according to current EEC directives.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(60)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method:
Year: **GLP:** no
Test substance:
Remark: Instillation into the conjunctival sac of 20 ug caused moderately severe irritation of the cornea.
Not classifiable according to current EEC directives.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(65)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method: Draize Test
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: 2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72 hrs), 0 (7 days).
Not classifiable according to current EEC directives.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(60)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method:
Year: **GLP:** no
Test substance:
Remark: Instillation into the conjunctival sac of 20 ug caused moderately severe irritation of the cornea.
Not classifiable according to current EEC directives.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(65)

5.3 Sensitization

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: other: Maximization test
Year: **GLP:** no
Test substance: no data
Remark: In an attempt to induce sensitization in 29 volunteers, subjects were given five 48-hr closed patch tests (during a 10-day period) with 4% in petrolatum. None of the subjects showed any positive reactions when challanged 10-14 days after the induction phase by final 48-hr closed patch test with the 4% petrolatum mixture.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(92)

5.4 Repeated Dose Toxicity

Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: inhalation
Exposure period: 90 days
Frequency of treatment: 6 hours/day, 5 days/week (total of 65 exposures)
Post. obs. period: none
Doses: 0, 15, 40 and 120 ppm
Control Group: yes
NOAEL: >= 120 ppm
Method: OECD Guide-line 413 "Subchronic Inhalation Toxicity: 90-day Study"
Year: 1981 **GLP:** yes
Test substance: other TS: purity 99.9%
Remark: 10 animals/sex/dose were used. The concentration of 120 ppm corresponds to the calculated saturated vapor concentration at 20?C. Body weights were determined weekly. Clinical signs and findings were recorded. Ophthalmologic examinations were carried out and blood was taken from all animals at the end of the 3-month exposure period. Nummerous clinicochemical and hematological parameters, and various enzyme activites were measured and a clotting time analysis wes performed. The animals were sacrificed at the end of the 3-month exposure period and a complete necrpsy of all animals including weighing of certain organs and a gross-pathologic evaluation was performed; selected organs/tissues were examined histologically.
Result: Under the conditions of the test no treatment-related toxic effects were found in male and female Wistar rats which were exposed to 2-ethylhexanol vapor up to 120 ppm.
Source: Neste Oxo AB Stenungsund
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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(93)

Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: inhalation
Exposure period: 90 Tage
Frequency of treatment: 6 Std./Tag, 5 Tage/Woche
Post. obs. period: keine
Doses: 0.081; 0.216; 0.648 mg/l (15; 40; 120 ppm) als Dampf
Control Group: yes
NOAEL: .648 mg/l
Method: OECD Guide-line 413 "Subchronic Inhalation Toxicity: 90-day Study"
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Je 10 maennliche und 10 weibliche Tiere wurden in die Kontroll- und Versuchsgruppen eingesetzt.
Es wurden in keiner Versuchsgruppe substanzbedingte Veraenderungen festgestellt. Untersucht wurden klinische, ophthalmologische, haematologische und klinisch-chemische Parameter. Nach Versuchsende wurden die Tiere pathologisch untersucht.
Source: BASF AG Ludwigshafen

(94)

Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: inhalation
Exposure period: 14 Tage
Frequency of treatment: 6 Std./Tag, 5 Tage/Woche
Post. obs. period: keine
Doses: 0.16; 0.32, 0.65 mg/l (30; 60; 120 ppm) als Dampf
Control Group: yes
NOAEL: .32 mg/l
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Es handelte sich um eine Range-finding-study fuer einen 90-Tageversuch. Keine substanzbedingten Veraenderungen wurden festgestellt, mit Ausnahme einer leichten Induktion der Cyanid-insensitiven Palmitoyl-CoA-Oxidase-Aktivitaet im Leberhomogenat der Tiere der hoechsten Dosisgruppe.
Source: BASF AG Ludwigshafen

(95)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 11 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 0, 0.46%, 0.92%, 1.38%, 2.75% microencapsulated 2-ethylhexanol in the diet
Control Group: yes
NOAEL: < .46 %
LOAEL: = .46 %
Method:
Year: **GLP:** yes
Test substance: other TS: purity 99.8%
Remark: Control: placebo microcapsules (3%9 in the diet.
Result: Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female rats per dose. The administration of 0.46, 0.92, 1.38 and 2.75 % (w/w) 2-ethylhexanol corresponded to a mean daily substance intake of about 500, 980, 1430, 2590 mg/kg bw 2-ethylhexanol in the male rat and of about 540, 1060, 1580, 2820 mg/kg body weight in the female rats. In all dose groups test substance related toxic effects were observed.
Typical findings were:

0.46% group:increased relative stomach weights in the females; decreased cholesterol in both sexes; decreased triglycerides and alanine-aminotransferase in the males.

0.92% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute stomach weights in the females; decreased triglycerides and alanine-aminotransferase and increased total protein in the males; minimal diffuse hypertrophy of the hepatocytes in one female; slight diffuse hypertrophy of the hepatocytes in all male and female rats.

1.38% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute liver weights in both male and female animals; increase in the absolute stomach weights in the females; decreased cholesterol in both sexes; decreased triglycerides and alanine-aminotransferase in the males and decreased platelets in the females; increased total protein in the males; slight diffuse hypertrophy of the hepatocytes in most male and female rats; focal or multifocal acanthosis in the epithelium of the forestomach of one female rat.

2.75% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute liver weights in the male and female animals; decreased cholesterol, triglycerides, glucose, alanine-aminotranferase, reticulocytes, platelets and mean corpuscular volume in both sexes; focal or multifocal acanthosis in the epithelium of the forestomach in a few

males and females.

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Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(96)

Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 3 weeks
Frequency of treatment: daily
Post. obs. period: none
Doses: 2% in the diet
Control Group: yes
Method:
Year: **GLP:**
Test substance: no data
Result: Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACTEYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.
Source: Neste Oxo AB Stenungsund

(97)

Species: rat **Sex:** male/female
Strain: other: Dow-Wistar
Route of admin.: oral feed
Exposure period: 3 months
Frequency of treatment: daily
Post. obs. period: none
Doses: 0.01, 0.05, 0.25, 1.25 % in the diet
Control Group: yes
NOAEL: = .05 %
LOAEL: = .25 %
Method:
Year: **GLP:** no
Test substance:
Result: Result: 10 male and 10 female rats per dose group were treated with 2-ethylhexanol. No mortality, appetite depression, body weight gain, or kidney weight effect was found associated with dosing. Typical findings were:

1.25% group: increased liver weights (absolute and relative) in both males and females; cortical degeneration of the kidney in the males; focal liver congestion and/or swelling in female rats; increased incidence and distribution of transitory hepatic diffuse cloudy swelling and also diffuse

cloudy swelling of the proximal convoluted kidney tubules.

0.25% group:A trend of the diffuse cloudy swelling of the liver and the kidney was suggested histologically although to a proportionally smaller degree, and believed to be fortuitous.

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(98)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 11 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine
Doses: 1; 2; 3; 6 % in Mikrokapseln im Futter entspr. 0.46; 0.92; 1.38; 2.75 % 2-Ethylhexanol
Control Group: yes, concurrent vehicle
NOAEL: < .46 %
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Kein Tier starb waehrend der Versuchsdauer. Die durchschnittliche taegliche Substanzaufnahme wurde fuer die weiblichen Tiere mit 500; 980; 1430 und 2590 mg/kg und fuer die maennlichen Tiere mit 540; 1060; 1580; 2820 mg/kg angegeben.
In der 6 % Dosisgruppe wurde eine verminderte Trinkwasser- und Futteraufnahme waehrend der Versuchsdauer beschrieben. Das Koerpergewicht der Tiere war reduziert.
Klinisch-chemische Untersuchungen erbrachten erniedrigte Werte von Cholesterol, Glucose und Alanin-Aminotransferase. Eine Abnahme von Reticulocyten, Thrombocyten und MCV wurde bei beiden Geschlechtern, von MCH bei weiblichen Tieren festgestellt. Ein Ansteigen des Gesamtproteingehaltes und der Erythrocyten wurde gemessen. Absolutes und relatives Lebergewicht waren erhoeht, wie auch das relative Magengewicht. Nur bei einem weiblichen Tier wurden makroskopisch fokale Laesionen im Vormagen festgestellt, mikroskopisch wurden bei mehreren Tieren Akanthose (fokal und multifokal) im Epithel des Vormagens beobachtet. Eine leichte diffuse Hypertrophie von Hepatocyten wurden bei allen Tieren dieser Dosisgruppe festgestellt.
Auch in der 3 % und 2 % Dosisgruppe wurden die klinischen, klinisch-chemischen und haematologischen Veraenderungen, wie auch die pathologischen Organveraenderungen der hoechsten Dosisgruppe festgestellt.

Auch in der 1 % Dosisgruppe wurde bei den maennlichen Tieren eine reduzierte Futteraufnahme beobachtet, auch waren die Veraenderungen bei den untersuchten klinisch-chemischen Parametern noch festzustellen. Bei den weiblichen Tieren war das relative Magengewicht erhoeht.
Aufgrund der Befunde muss der NOAEL unterhalb der niedrigsten Dosierung liegen, d.h. < 0.46 % 2-Ethylhexanol.

Source: BASF AG Ludwigshafen

(99)

Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 3 weeks
Frequency of treatment: daily
Post. obs. period: none
Doses: 2% in the diet
Control Group: yes
Method:
Year: **GLP:**
Test substance: no data
Result: Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACTEYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.
Source: Neste Oxo AB Stenungsund
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Hoechst AG Frankfurt/Main

(100)

Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 3 weeks
Frequency of treatment: daily
Post. obs. period: none
Doses: 2% in the diet
Control Group: yes
Method:
Year: **GLP:**
Test substance: no data
Result: Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACTEYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(100)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: drinking water
Exposure period: 9 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 0, 308, 636 ppm
Control Group: yes, concurrent vehicle
NOAEL: = 636 ppm
Method: other: according to TSCA and EPA guidelines
Year: 1983 **GLP:** yes
Test substance: other TS: purity >99.5%
Result: Result: Per dose, groups of 10 male and 10 female rats were exposed to 2-ethylhexanol. There were no treatment-related effects on clinical signs of toxicity, food consumption, body weight, serum chemistry, hematology, organ weights, gross pathology, or anatomic pathology.
Source: Neste Oxo AB Stenungsund
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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(101)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 21 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 100, 300, 950 mg/kg/day (vehicle:corn oil)
Control Group: yes, concurrent vehicle
LOAEL: 100 mg/kg
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Result: Result: Subchronic toxicity was elvaluated in groups of 5 female and 5 male rats. There were no mortalities.

Clinical observations included reduced body weight gain in high dose females. Necropsy revealed elevated absolute and realtive liver weights in high dose males and females in the 2 highest dose groups; elevated realtive kidney weights in high dose females and males; increased serum triglyceride levels in high dose males; increased lauric acid 11-and 12-hydroxylase activities in high dose females and males; a dose related reduction in neutral lipids in the livers of treated animals; a dose related increase in cyanide-insensitive palmitoyl CoA oxidation in females and males; slightly increased hepatic peroxisomes in high dose

females and males.

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(102)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 3 months
Frequency of treatment: daily (5 days /week)
Post. obs. period: none
Doses: 25, 125, 250, 500 mg/kg (in aqueous emulsion)
Control Group: yes, concurrent vehicle
NOAEL: = 125 mg/kg
LOAEL: = 250 mg/kg
Method:
Year: **GLP:** yes
Test substance: other TS: purity >99.8%
Remark: Vehicle: bidistilled water containing 5 ug/ml Cremophor EL. Concurrently to the main study a limited study with the same dosing regimen using 3 animals/sex/dose was performed; at the end of the treatment period all animals were sacrificed and samples of liver tissues and bone marrow were prepared for electron microscopy investigations; liver homogenates were prepared for clinicochemical examinations;
Result: Result:
Limited study:

The oral administration of 2-ethylhexanol over a period of 3 months led to an impairment of feed consumption and body weight gain in the male and female animals of the 500 mg/kg dose group. The cyanide-insensitive palmitoyl CoA-oxidation in the liver of male and female rats was strongly induced in the 500 mg/kg dose group and less pronounced in the 250 mg/kg dose group, probably due to a proliferation of peroxisomes. No substance-related findings were observed in the other dose groups.
NOEL: 125 mg/kg bodyweight
LOEL: 250 mg/kg bodyweight

Main study:

Per dose group 10 male and 10 female rats were treated. After the 3-month administration of 2-ethylhexanol toxic effects occurred in male and female rats of the 500 and 250 mg/kg dose groups. Typical findings were:

25 and 125 mg/kg groups: no substance-related findings

250 mg/kg group: increased relative liver weights in both sexes; increased relative stomach weights in females; decrease in alkaline phosphatase and glucose in males; decrease in alanine-aminotransferase in female rats.

500 mg/kg group: increased relative liver and stomach weights in both sexes; increased relative liver weights in the animals of both sexes; increased absolute stomach weights in female rats; decrease in alanine-aminotransferase, glucose and cholesterol in both sexes; decrease in alkaline phosphatase in males; single or multiple slightly elevated foci in the mucosa of the forestomach of male and female rats; focal or multifocal acantosis in the mucosa of the forestomach of one male and five female animals.

Source: Neste Oxo AB Stenungsund
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(103)

Species: rat **Sex:** male
Strain: Wistar
Route of admin.: gavage
Exposure period: 7 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 0, 1335 mg/kg/day in corn oil
Control Group: yes, concurrent vehicle
Method:
Year: **GLP:** no
Test substance: no data
Result: Result: The oral administration of 1335 mg/kg 2-ethylhexanol to a group of 6 male Wistar rats resulted in increased relative liver weights as compared to the control. In addition, significantly increased activity of cytochrome P-459s and biphenyl-4-hydroxylase of the liver were observed. Microsomal glucose-6-phosphatase activity was significantly decreased, while liver succinate dehydrogenase and aniline-4-hydroxylase activities were similar to the control. In the liver, electronmicroscopy studies showed and increase in the number of peroxisomes and dilatation of the smooth endoplasmic reticulum.

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(104)

Species: rat **Sex:** male
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 5 days
Frequency of treatment: daily
Post. obs. period:
Doses: 352 mg/kg
Control Group:
Method:
Year: **GLP:**
Test substance:
Result: Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.
Source: Neste Oxo AB Stenungsund

(105)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 11 days (9 applications)
Frequency of treatment: 5 days/week
Post. obs. period: none
Doses: 0, 100, 330, 1000, 1500 mg/kg (in aqueous emulsion)
Control Group: yes, concurrent vehicle
NOAEL: = 100 mg/kg
LOAEL: 330 mg/kg
Method:
Year: **GLP:** yes
Test substance: other TS: purity >99.8%
Remark: vehicle: bidistilled water containing 5 ul/100 ml Cremophor EL.
Result: Result:Per dose 10 male and 10 female animals were treated. The 9-fold administration of 2-ethylhexanol to rats at doses of 1000 and 1500 mg/kg body weight led to clear toxic signs like impairment of food consumption and body weight gain as well as ataxia and/or lethargy. No substance-related effects were observed in the 100 mg/kg dose group.

1500 mg/kg dose group:
decrease of cholesterol, glucose and reticulocytes in the animal of both sexes; increase of alanine aminotransferase in the males; increased relative stomach, liver , kidney and brain weights and decreased relative spleen weights in both sexes; increased relative adrenal weight in the male and lung weight in the female animals; foci in the forestomach of 4 male and 7 female animals; hyperkeratosis and focal or multifocal acanthosis in the mucuos membrane of the forestomac of all rats as well as epithelial degeneration,

ulceration and subcutaneous inflammatory edema in some animals; slight hypertrophy of hepatocytes in the liver of 8 male and female rats each; focal hepatocellular necrosis in 2 male and 1 female rat; parenchymal involution of lympho-reticular tissue in the spleen in both sexes; decreased thymus size and lymphocyte depletion and necrosis in animals of both sexes.

1000 mg/kg dose group:
decrease of cholesterol and reticulocytes in both sexes; increased relative stomach, liver and kidney weights and decreased spleen weights in both sexes; increased relative brain weight in the femal rats; foci in the forestomach of 2 males; hyperkeratosis and focal or multifocal acantosis in the mucous membrande of the forestomach of most male and female rats as well as epithelial degeneration, ulceration and subcutaneous inflammatory edema; parenchymal involution of lymphoreticular tissue in the spleen of 5 female rats, decreased thymus size in 2 male and 5 female rats; lymphocyte depletion and necrosis in the thymus of some female rats.

330 mg/kg dose group:
increased relative kidney weights of the female rats; inflammatory edema in the forestomach of 1 female and decreased thymus size in 2 male and 1 female rat.

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(106)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 9 days
Frequency of treatment: 5 days + 2 days without treatment + 4 days
Post. obs. period: none
Doses: 0.1, 0.33, 1.0, 1.5 ml/kg/day (=83, 275, 834, 1250 mg/kg/day)
Control Group: yes
NOAEL: 83 mg/kg
Method: other: according to TSCA and EPA guidelines
Year: 1983 **GLP:** yes
Test substance: other TS: purity >99.5%
Result: Result: Per dose, groups of 10 male and 10 female F-344 rats were exposed by oral gavage to 2-ethylhexanol (undiluted). Treatment resulted in a spectrum of treatment-related, dose-dependent toxic effects in male and female rats.

No treatment-related effects were observed for any in-life, clinical pathology, gross necropsy, or histopathology

observations at the 0.1 ml/kg/day level.

Effects associated with the administration of 2-ethylhexanol in males and/or females at one or more of the three highest dose levels were decreased food consumption and body weights, decreased total leukocytes and lymphocytes, increased liver weight, increased stomach weight (associated with hyperkeratosis, mucosal hyperplasia, edema, exocytosis and gastritis of the forestomach, but not glandular stomach), decreased spleen weight, thymic atrophy and lymphoid cell degeneratiion.

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(101)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 11 days (9 applications)
Frequency of treatment: 5 days/week
Post. obs. period: none
Doses: 0, 100, 330, 1000, 1500 mg/kg (in propylene glycol)
Control Group: yes, concurrent vehicle
NOAEL: < 100 mg/kg
LOAEL: = 100 mg/kg
Method:
Year: **GLP:** yes
Test substance: other TS: purity >99.8%
Remark: Vehicle: propylene glycol
Result: Per dose group, 10 male and 10 female rats were treated. 1500 mg/kg b.w. 2-ethylhexanol proved to be lethal for all female animals and 6 of the male animals. Doses of 1500, 1000, and 330 mg/kg bw resulted in clinically observable toxic effects like lethargy, ataxia, and/or reduced food consumption accompanied by reduced body weight gain.

1500 mg/kg group:
Extremly reduced feed consumption and body weight in the surviving males; decrease of cholesterol, alanine-aminotransferase, leucocytes, lymphocytes, monocytes, hemoglobin, hematocrit, meancell volume, mean corpuscular hemoglobin and reticulocytes; increase in neutrophilic polymorpho-nuclear granulocytes; increase in relative stomach, liver and kidney weights and decrease in relative spleen and testes weights; foci in the forestomach.

1000 mg/kg dose group:
Reduced feed consumption and body weight in the animals of both sexes; decrease of cholesterol,

alanine-aminotransferase, leucocytes, lymphocytes, monocytes, hemoglobin, hematocrit, mean cell volume and reticulocytes and increaseof the neutrophilic polymorphonuclear granulocytes in both sexes; decrease of the mean corpuscular hemoglobin in the males; increased relative stomach, liver and kidney and decreased relative spleen weights in both sexes; increased testes weights in males; foci in the forestomach of all animals and ulcer in the forestomach of 2 males.

330 mg/kg group:
Decrease of alanine-aminotransferase, hemoglobin, hematocrit, mean cell volume and reticulocytes and increase in the neutrophilic polymorphonuclear granulocytes in the females: increased relative stomach weight in both sexes, increased relative liver weight in the female and increased testes weights in the male animals; foci in the forestomach of all animals.

100 mg/kg group:
Decreased of alanine-aminotransferase in the females; decreased relative liver weights in the male animals.

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(107)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 11 days (9 applications)
Frequency of treatment: 5 days /week
Post. obs. period: none
Doses: 100, 330, 1000, 1500 mg/kg (in corn oil)
Control Group: yes, concurrent vehicle
NOAEL: = 100 mg/kg
LOAEL: = 330 mg/kg
Method:
Year: **GLP:** yes
Test substance: other TS: purity >99.8%
Result: Per dose 10 male and 10 female animals were treated. The 9-fold administration of 2-ethylhexanol to rats at doses of 1000 and 1500 mg/kg bw led to clear toxic signs like impairment of food consumption and body weight gain as well as ataxia and/or lethargy, piloerection, and genital region smeared with urine in both sexes. Some of these toxic signs were also found in some animals of the 330 mg/kg dose group.

1500 mg/kg dose group:
One female rat died during the conduct of the study;

decrease of cholesterol, glucose, alanine-aminotransferase, leukocytes, lymphocytes, monocytes and reticulocytes in both sexes; lowering of mean cell volume and mean corpuscular hemoglobin in the females; increase in total protein and triglycerides in both sexes; increased relative stomach, liver and kidney and decreased relative spleen weights in both sexes; increased relative testes weights; thickening of the wall of the forestomach and foci in the forestomach in some males and females.

1000 mg/kg dose group:
One male rat died during the conduct of the study; decrease of cholesterol, glucose, leukocytes, lymphocytes and reticulocytes in both sexes; decrease of monocytes and increase of total protein in the males and decrease of themean cell volume in the females; increased relative stomach,liver and kidney and decreased relative spleen weights in both sexes; increased relative testes weights; thickening of the wall and foci in the forestomach in some animals.

330 mg/kg dose group:
Increased relative testes weights; thickening of the wall and foci in the forestomach in some animals.

100 mg/kg dose group:
No substance-related findings.

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Celanese GmbH Frankfurt am Main

(108)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 11 Tage
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 100; 330; 1000; 1500 mg/kg in Maisoel appliziert
Control Group: yes, concurrent vehicle
NOAEL: 100 - 330 mg/kg
LOAEL: 330 mg/kg
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Testsubstanz wurde in 5 ml/kg Maisoel appliziert. In der 1500 mg/kg Dosisgruppe starb ein weibliches Tier waehrend der Versuchsdauer, in der 1000 mg/kg Dosisgruppe ein maennliches Tier.

In der hoechsten Dosisgruppe waren Futteraufnahme und Koerpergewichtsentwicklung reduziert. Ataxie, gestraeubtes Fell und bei einigen Tieren Lethargie und Speichelfluss wurden beobachtet. Bei 9 weiblichen Tieren und einem maennlichen Tier war in der Genitalregion das Fell mit Urin verklebt. Klinisch-chemische und haematologische Untersuchungen zeigten reduzierte Cholesterin-, Glucose- und Alanin-Aminotransferase-Werte. Gesamtproteingehalt und Triglyceride waren erhoeht. Leukocyten-, Lymphocyten-, Monocyten und Reticulocytenzahl war verringert, bei den weiblichen Tieren war auch das mittlere Blutkoerperchenvolumen und der Hb-Faerbkoeffizient verringert. Die absoluten Organgewichte von Leber und Milz waren bei beiden Geschlechtern reduziert, die von Niere und Hoden waren bei den maennlichen Tieren reduziert, vom Magen erhoeht. Relativ waren Magen-, Leber- und Nierengewicht bei beiden Geschlechtern erhoeht und Milzgewicht verringert. Das relative Hodengewicht war erhoeht. Histologisch wurde eine Verdickung der Vormagenwand, bei einigen Tieren mit Focibildung, beschrieben.
In der 1000 mg/kg Dosisgruppe wurden im wesentlichen noch die gleichen Symptome wie in der 1500 mg/kg Dosisgruppe beobachtet.
330 mg/kg bewirkten Ataxie, gestraeubtes Fell und Urin auf dem Fell im Genitalbereich nur noch bei einigen Tieren. Es wurden keine klinisch-chemischen wie auch haematologischen Veraenderungen festgestellt. Das relative Hodengewicht war erhoeht. Die Veraenderungen im Vormagen wurden nur noch bei 3 Tieren festgestellt.
Bei den Tieren, die 100 mg/kg erhielten wurden keine substanzbedingten Veraenderungen festgestellt.

Source: BASF AG Ludwigshafen

(109)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 11 Tage
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 100; 330; 1000; 1500 mg/kg in Propylenglykol appliziert
Control Group: yes, concurrent vehicle
NOAEL: < 100 mg/kg
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Je 10 maennliche und 10 weibliche Tiere wurden in die Versuchs- und Kontrollgruppen eingesetzt. Die Substanz wurde in je 5 ml/kg Propylenglykol appliziert.
In der 1500 mg/kg Dosisgruppe starben alle weiblichen und 6 maennliche Tiere. Die Futteraufnahme und die Koerpergewichtsentwicklung der ueberlebenden Tiere war signifikant reduziert, die Trinkwasseraufnahme erhoeht. Ataxie, Lethargie, gestraeubtes Fell, Bewusstseinsverlust, Hypothermie und bei einigen Tieren Speichelfluss und Urin

auf dem Fell im Genitalbereich wurden als klinische Veraenderungen beschrieben. Bei den ueberlebenden Tieren waren im Blut Cholesterin, die Alanin-Aminotransferase, Leukocyten, Lymphocyten, Monocyten, Haemoglobin, Haematokrit, MCV und MCH reduziert, neutrophile polymorphkernige Granulocyten erhoeht. Die relativen Magen-, Leber- und Nierengewichte waren erhoeht, relative Hoden- und Milzgewichte verringert. Absolut waren Magen- und Lebergewichte erhoeht, Milz- und Nierengewichte reduziert. Bei allen ueberlebenden Tieren wurden Foci im Vormagen festgestellt.
2 Tiere der 1000 mg/kg Dosisgruppe starben.
Klinische, klinisch-chemische und haematologische Veraenderungen entsprachen im wesentlichen denen, die bei den ueberlebenden Tieren der 1500 mg/kg Dosisgruppe beschrieben wurden.
In der 330 mg/kg Dosisgruppe wurden bei je 3 maennlichen und 3 weiblichen Tieren noch klinische Veraenderungen in Form von Ataxie und Lethargie beschrieben. Auch waren die klinisch-chemischen und haematologischen Parameter noch veraendert. Absolute und relative Magen- und Hodengewichte waren erhoeht, wie auch die relativen Lebergewichte bei weiblichen Tieren. Bei allen Tieren wurde Focibildung im Vormagen beschrieben.
In der 100 mg/kg Dosisgruppe waren bei den weiblichen Tieren die Alanin-Aminotransferase vermindert. Bei den maennlichen Tieren wurden verringerte relative Lebergewichte beschrieben. Keine weiteren substanzbedingten Veraenderungen wurden festgestellt.
Der NOEAL liegt unter 100 mg/kg.

Source: BASF AG Ludwigshafen

(110)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 11 Tage
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 100; 330; 1000; 1500 mg/kg in waessriger Emulsion appliziert
Control Group: yes, concurrent vehicle
NOAEL: 100 - 330 mg/kg
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Je 10 maennliche und 10 weibliche Tiere wurden in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert dem 5 ul/100 ml Cremophor EL zugesetzt waren.
Kein Tier starb waehrend der Versuchsdauer.
In der 1500 mg/kg Dosisgruppe war die Futteraufnahme und das Koerpergewicht der Tiere reduziert. Klinische Veraenderungen waren Ataxie, Lethargie, z.T. erschienen die Tiere bewusstlos, gestraeubtes Fell und Urin auf dem Fell im Genitalbereich. Die Cholesterol- und Glucosewerte waren

reduziert, die Alanin-Aminotransferase bei den maennlichen Tieren erhoeht. Die Reticulocytenzahl war vermindert. Das absolute Organgewicht von Milz, Gehirn und Nebenniere war reduziert, das von Leber und Magen erhoeht. Relativ waren Magen-, Nieren-, Leber- und Gehirngewicht erhoeht, das relative Nebennierengewicht war bei den maennlichen Tieren und das relative Lungengewicht bei den weiblichen Tieren erhoeht. Das relative Milzgewicht war bei beiden Geschlechtern reduziert. Makroskopisch wurden im Vormagen bei den meisten Tieren Foci festgestellt. Histologisch wurden Hyperkeratosen, Akanthosen (fokal, multifokal) in der Vormagenschleimhaut bei allen Tieren beschrieben, bei einigen Tieren wurden epitheliale Degenerationen, Ulcerationen und subkutane entzuendliche Oedeme beschrieben. Bei einigen Tieren wurde eine leicht Hypertrophie der Hepatocyten, fokale hepatocellulaere Nekrosen und eine Rueckbildung des lymphoreticularen Gewebes festgestellt. Eine Verminderung der Thymusgroesse wurde bei fast allen Tieren beobachtet, wie auch eine Lymphocytendepletion im Thymus, bei einigen Tieren Lymphocytennekrosen.
In der 1000 mg/kg Dosisgruppe wurden die gleichen Veraenderungen wie in der hoechsten Dosisgruppe beschrieben.
In der 330 mg/kg Dosisgruppe waren die relativen Nierengewichte der weiblichen Tiere erhoeht. Die Thymusgroesse war bei 3 Tieren vermindert, bei einem weiblichen Tier wurden entzuendliche Oedeme im Vormagen festgestellt. Keine weiteren substanzbedingten Veraenderungen wurden beschrieben.
100 mg/kg bewirkte keine substanzbedingten Effekte.

Source: BASF AG Ludwigshafen

(111)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 3 Monate
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 25; 125; 250; 500 mg/kg als waessrige Emulsion appliziert
Control Group: yes, concurrent vehicle
NOAEL: 125 - 250 mg/kg
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Je 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg Wasser appliziert, dem 5 ul/100 ml Cremophor EL zugesetzt waren. Keine Tiere starben waehrend der Versuchsdauer.
In der hoechsten Dosisgruppe war sowohl die Koerpergewichtsentwicklung wie auch das Koerpergewicht der Tiere reduziert. Alanin-Aminotransferase, Glucose- und Cholesterolspiegel waren vermindert bei beiden Geschlechtern, bei den maennlichen Tieren war die alkalische Phosphatase vermindert, der Gesamtprotein- und Albumingehalt

erhoeht. Ein Ansteigen der Reticulocyten wurde beschrieben. Absolute und relative Magen- und Lebergewichte waren erhoeht. Focibildung in der Schleimhaut des Vormagens wurde beschrieben. Histologisch wurden bei einigen Tieren Akanthose der Mucosa im Vormagen beschrieben. Bei einigen Tieren traten fettige Infiltrationen in der Leber (lobulaere Peripherie) auf.
In der 250 mg/kg Dosisgruppe wurden keine klinischen Veraenderungen festgestellt. Bei den maennlichen Tieren waren die alkalische Phosphatase und der Glucosespiegel reduziert, bei weiblichen Tieren die Alanin-Aminotransferase erhoeht. Das relative Lebergewicht war bei beiden Geschlechteren erhoeht, das relative Magengewicht nur bei weiblichen Tieren. Bei mikroskopischen Untersuchungen wurden geringgradige Fetteinlagerungen in den Leberzellen festgestellt.
In der 125 und 25 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.

Es wurde zusaetzlich eine Satellitenstudie mit je 3 maennlichen und weiblichen Tieren pro Versuchs- und Kontrollgruppe durchgefuehrt. Bei diesen Tieren wurde nach Versuchsende das Leber- und Knochenmarkgewebe fuer elektronenmikroskopischen Untersuchungen praepariert. Sowohl in der 250 wie auch 500 mg/kg wurde bei beiden Geschlechtern dosisabhaengig eine Induktion der Cyanid-resistenten (peroxisomalen) Palmitoyl-CoA-Oxidase festgestellt.

Source: BASF AG Ludwigshafen

(112) (113)

Species: rat **Sex:** male
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 5 days
Frequency of treatment: daily
Post. obs. period:
Doses: 352 mg/kg
Control Group:
Method:
Year: **GLP:**
Test substance:
Result: Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(114)

Species: rat **Sex:** male
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 5 days
Frequency of treatment: daily
Post. obs. period:
Doses: 352 mg/kg
Control Group:
Method:
Year: **GLP:**
Test substance:
Result: Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(114)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: dermal
Exposure period: 9 days
Frequency of treatment: 5 days treatment, 2 days no treatment, 4 days treatment
Post. obs. period: none
Doses: 0, 0.5, 1.0 ml/kg/day (=0, 417, 834 mg/kg/day)
Control Group: yes
Method: other: according to TSCA and EPA guidelines
Year: 1983 **GLP:** yes
Test substance: other TS: purity >99.5%
Remark: Control: water
Result: Result: Per dose, groups of 10 male and 10 female F-344 rats were exposed to 2-ethylhexanol (undiluted, occluded cutaneous). Exposure was for 6 hours per treatment day. There were no treatment-related effects on clinical signs of toxicity, food consumption, or body weight following cutaeous exposure to 2-ethylhexanol. Lymphopenia and decreased spleen weight for high dose females and increased triglycerides for females at both dose levels compared to controls were observed. No other treatment-related effects on clinical pathology measurements or organ weights were observed for males or females at either dose level. Treatment-related anatomic and histologic lesions observed following cutaneous exposure to 2-ethylhexanol were restricted to the site of application and included exfoliation, acanthosis, hyperkeratosis, eschar formation, dermatitis and edema.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(101)

Species: rat **Sex:** male
Strain: other
Route of admin.: dermal
Exposure period: 16 days
Frequency of treatment: 5 days/week
Post. obs. period: 14 days
Doses: 0, 2.0 ml/kg/day
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:** no
Test substance:
Result: Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period).

On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced.

There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum.

Histologically the following effects on organs were observed (with at least 3 out of 5 treated animals differing from the controls):

Liver: histiocytic and inflammatory granulomas, peripheral fine-droplet fatty degeneration.
Lungs: interstitial pneumonia, bronchiectasis, severe round-cell bronchitis.
Kidneys: Epithelial-cell necrosis, cysts, basophilic "ballon nuclei".
Heart: inter- and intracellular oedema, necrobiotic muscle fibres, interstitial oedema.
Testes: interstitial oedema, reduced spermiogenesis.
Thymus: increased "colliodocytes".
Adrenals: Cortex very rich in lipoids.

Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.

Source: Neste Oxo AB Stenungsund

(115)

Species: rat **Sex:** male
Strain: other
Route of admin.: dermal
Exposure period: 16 days
Frequency of treatment: 5 days/week
Post. obs. period: 14 days
Doses: 0, 2.0 ml/kg/day
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:** no
Test substance:
Result: Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period).

On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced.

There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum.

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Adrenals: Cortex very rich in lipoids.

Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(81)

Species: rat **Sex:** male
Strain: other
Route of admin.: dermal
Exposure period: 16 days
Frequency of treatment: 5 days/week
Post. obs. period: 14 days
Doses: 0, 2.0 ml/kg/day
Control Group: yes, concurrent no treatment
Method:
Year: **GLP:** no
Test substance:
Result: Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period).

On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced.

There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum.

Histologically the following effects on organs were observed (with at least 3 out of 5 treated animals differing from the controls):

Liver: histiocytic and inflammatory granulomas, peripheral fine-droplet fatty degeneration.
Lungs: interstitial pneumonia, bronchiectasis, severe round-cell bronchitis.
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Heart: inter- and intracellular oedema, necrobiotic muscle fibres, interstitial oedema.
Testes: interstitial oedema, reduced spermiogenesis.
Thymus: increased "colliodocytes".
Adrenals: Cortex very rich in lipoids.

Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(81)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 11 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 0.22, 0.44, 0.66, 1.32 % microencapsulated in the diet
Control Group: yes, concurrent vehicle
NOAEL: = .44 - .66 %
LOAEL: = .66 - 1.32 %
Method:
Year: **GLP:** yes
Test substance: other TS: purity >99.8%
Remark: NOEL: 0.44% = 1150 mg/kg/d (males)
0.66% = 2650 mg/kg/d (females)

Control: placebo microcapsules (1.5%) in the diet.
Result: Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose. The administration of 0.22, 0.44, 0.66 and 1.32 % 2-ethylhexanol in the diet corresponded to a mean daily intake of about 550, 1150, 1800 and 4450 mg/kg b w 2-ethylhexanol for male mice and of about 750, 1750, 2650 and 5750 mg/kg bw for female mice. The only effect that could be assessed to be a substance related finding was the reduction in body weight gain in the male animals of the 0.66% group.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(116)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 11 Tage
Frequency of treatment: kontinuierlich
Post. obs. period: keine
Doses: 0.48; 0.96; 1.44; 2.88 % in Mikrokapseln im Futter, entspr. 0.22; 0.44; 0.66; 1.32 % 2-Ethylhexanol
Control Group: yes, concurrent vehicle
NOAEL: .44 - .66 %
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Es wurden je 10 maennliche und 10 weibliche Tiere in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanzaufnahme wurde fuer die weiblichen Tiere mit 750; 1750; 2650 und 5750 mg/kg angegeben, fuer die maennlichen Tiere mit 550; 1150; 1800 und 4450 mg/kg.
Kein Tier starb waehrend der Versuchsdauer. In der hoechsten Dosisgruppe wurde bei beiden Geschlechtern eine verminderte Koerpergewichtsentwicklung festgestellt, in der zweithoechsten Dosierung wurde dieses nur noch bei den maennlichen Tieren beobachtet. Es traten keine weiteren substanzbedingten Veraenderungen auf, untersucht wurden sowohl klinisch-chemisch und haematologisch Parameter, wie auch moegliche Organveraenderungen.
Der NOEL wurde von den Autoren zwischen 0.44 und 0.66 % fuer maennliche Tiere und zwischen 0.66 und 1.32 % fuer weibliche Tiere angegeben. Der NOAEL liegt bei 1.32 % 2-Ethylhexanol.
Source: BASF AG Ludwigshafen

(117)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 11 days (9 applications)
Frequency of treatment: daily (9 applications)
Post. obs. period: none
Doses: 0, 100, 330, 1000, 1500 mg/kg (in corn oil)
Control Group: yes, concurrent vehicle
NOAEL: = 330 - 1000 mg/kg bw
LOAEL: = 1000 - 1500 mg/kg bw
Method:
Year: **GLP:** yes
Test substance: other TS: purity >99.8%
Remark: NOEL: 330 mg/kg (males)
1000 mg/kg (females)
Result: Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose.
In the 1500 mg/kg dose group 1 male mouse died, 10 male and 5 female mice had clinical signs as ataxia, piloerection and lethargy. A few animals showed abdomnial position and loss of consciousness. An increase in the absolute and relative

stomach weights was observed in male and female mice. In addition, male mice had decreased absolute and relative testes weights, and the relative liver and kidney weights of female mice were decreased.Gross lesions (foci in the mucosa) were seen in the forestomach of 7 male and 2 female mice.

In the 1000 mg/kg dose group, a decrease in absolute and relative testes weights was observed.

In the 100 and 330 mg/kg groups no substance-related findings were observed.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(118)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 3 months
Frequency of treatment: 5 days per week
Post. obs. period: none
Doses: 25, 125, 250, 500 mg/kg (aqueous emulsion)
Control Group: yes, concurrent vehicle
NOAEL: = 125 - 250 mg/kg
LOAEL: 250 - 500 mg/kg
Method:
Year: **GLP:** yes
Test substance:
Remark: Vehicle: bidistilled water containing 5 ug/100 ml Cremophore EL.
Concurrently to the main study a limited study with the same dosing regimen using 3 animals/sex/dose was performed; at the end of the treatment period all animals were sacrificed for electron microscopic investigations; liver homogenates were prepared for clinicochemical examinations.
Result: Results:

Limited study: At the end of the 3-month administration period there were no substance-related clinical findings. There was no increase in the activity of the cyanide-insensitive palmitoyl-CoA-oxidation in the liver of the animals in all dose groups.

Main study: NOEL (females) = 250 mg/kg
NOEL (males) =125 mg/kg

2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose. After the 3-month administration of

2-ethylhexanol toxic effects affecting the stomach (increased weight and slight focal and multifocal acanthosis in the mucosa of the forestomach) occurred in the male and female animals of the 500 mg/kg dose group and in the male animals (increased relative weight) of the 250 mg/kg dose group. Clinically, none of the animals showed any abnormal signs which could be related to the test substance administration.No substance-related effects occurred regarding the clinical chemistry or hematology.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(119)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 11 days (9 applications)
Frequency of treatment: 5 days/week
Post. obs. period: none
Doses: 0, 100, 330, 1000, 1500 mg/kg in propylene glycol
Control Group: yes, concurrent vehicle
NOAEL: = 100 mg/kg
LOAEL: = 330 mg/kg
Method:
Year: **GLP:** yes
Test substance: other TS: purity >99.8%
Result: Per dose group, 10 male and 10 female animals were treated. 1500 mg/kg and 1000 mg/kg 2-ethylhexanol being administered for 11 days (9 applications) proved to be a lethal dose for 4 male and 6 female (1500 mg/kg) or for 1 male and 1 female animal (1000 mg/kg), respectively. Doses of 1500 and 1000 mg/kg body weight resulted in clinically observable toxic effects like lethargy, ataxia, and/or reduced food consumption. Clinical chemistry and hematology did not show changes that could be related to the test substance administration.

1500 mg/kg dose group:
Increase relative stomach and liver weights in both sexes;increased relative spleen weight in female and decreased testes weights in the male mice; gross lesions (foci of the mucosa, mainly white colored and slightly prominent) in the forestomach of the surviving animals of both sexes.

1000 mg/kg dose group:
Increased relative stomach and liver weights in both sexes; increased relative spleen weights in males; gross lesion (foci of the mucosa, mainly white colored and slightly

prominent) in the forestomach of the surviving animals of both sexes.

330 mg/kg dose group:
Increased relative stomach and liver weights in the males; gross lesions (foci of the mucosa, mainly white colored and slightly prominent) in the forestomach of both sexes.

100 mg/kg dose group:
No substance-related findings

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(120)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 11 days (9 applications)
Frequency of treatment: 5 days/week
Post. obs. period: none
Doses: 0, 100, 330, 1000, 1500 mg/kg (aqueous emulsion)
Control Group: yes, concurrent vehicle
NOAEL: = 100 mg/kg
LOAEL: = 330 mg/kg
Method:
Year: **GLP:** yes
Test substance: other TS: >99.8%
Remark: Vehicle: bidistilled water containing 5 ug/100ml Cremophor EL
Result: Per dose group, 10 male and 10 female animals were treated. The 9-fold application of 2-ethylhexanol led to substance induced clinical signs like ataxia and/or abnormal position in the male animals of the 330 mg/kg and 1500 mg/kg groups and in the female animals of the 1000 mg/kg and 1500 mg/kg groups. 1 male and 4 female mice of the 1500 mg/kg dose group and 1 female mouse of the 1000 mg/kg dose group died during the study. Clinical chemistry and hematology revealed no changes that could be attributed to the test substance.

1500 mg/kg dose group:
Increase in relative stomach and liver weights in both sexes; foci in the forestomach of males and females; hyperkeratosis and focal or multifocal acanthosis and inflammatory edema in the submucosa of the forestomach as well as focal or multifocal ulceration of the mucous membrane in animals of both sexes; hypertophy of the hepatocytes in the liver in both sexes and focal necrosis of liver cells in one animal of both sexes: tubular giant cells in the testicular tubules in two male mice; tubular dilation

and nephrosis in the renal cortex of animals that died intercurrently and centrilobular fatty infiltration in the liver of intercurrently died females.

1000 mg/kg dose group:
Increased relative liver weights in male and stomach weights in female mice; foci in the forestomach of some animals of both sexes; hyperkeratosis and focal or multifocal acanthosis and inflammatory edema in the submucosa of the forestomach as well as focal or multifocal ulceration of the mucous membrane in animals of both sexes; hypertrophy of hepatocytes in one male and one female animal; tubular dilation in the renal cortex and centrilobular fatty infiltration in the liver of the female mouse which died intercurrently.

330 mg/kg dose group:
Acanthosis in the mucous membrane of the forestomach of 2 male and 2 female mice, mostly connected with hyperkeratosis in the submucosa.

100 mg/kg dose group:
No substance-related findings.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(121)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 11 Tage
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 100; 330; 1000; 1500 mg/kg in Maisoel appliziert
Control Group: yes, concurrent vehicle
NOAEL: 330 - 1000 mg/kg
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: 10 weibliche und 10 maennliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in je 5 ml/kg Maisoel appliziert.
In der 1500 mg/kg Dosisgruppe starb ein maennliches Tier waehrend der Versuchsdauer. Kein Effekt auf die Koerpergewichtsentwicklung wurde festgestellt. Bei allen maennlichen und 5 weiblichen Tieren dieser Dosisgrupppe wurde Ataxie, gestraeubtes Fell, Lethargie und bei einigen Tieren Bewusstlosigkeit beschrieben. Klinisch-chemische und haematologische Untersuchungen zeigten keine Veraenderungen.

Die absoluten Organgewichte vom Magen waren erhoeht, die der Hoden verringert. Auch die relativen Hodengewichte waren verringert, erhoeht waren die relativen Nieren- und Lebergewichte bei weiblichen Tieren und die relativen Magengewichte bei beiden Geschlechtern. Laesionen des Vormagens wurden bei 7 maennlichen und 2 weiblichen Tieren festgestellt.
In der 1000 mg/kg Dosisgruppe wurden bei den maennlichen Tieren verringerte absolute und relative Hodengewichte beschrieben, keine weiteren Veraenderungen wurden festgestellt.
In den beiden niederen Dosisgruppen wurden keine substanzbedingten Veraenderungen festgestellt.
Der NOAEL wurde fuer die maennlichen Tiere zwischen 330 und 1000 mg/kg angegeben, fuer die weiblichen Tiere zwischen 1000 und 1500 mg/kg.

Source: BASF AG Ludwigshafen

(122)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 11 Tage
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 100; 330; 1000; 1500 mg/kg appliziert in Propylenglykol
Control Group: yes, concurrent vehicle
NOAEL: 100 - 330 mg/kg
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Je 10 weibliche und 10 maennliche Tiere wurde pro Dosis- und Kontrollgruppe eingesetzt. Die Substanz wurde in 5 ml/kg Propylenglykol appliziert.
In der hoechsten Dosisgruppe starben 4 maennliche und 6 weibliche Tiere waehrend der Versuchsdauer. Bei den maennlichen Tiere wurde ein reduzierte Futteraufnahme, bei beiden Geschlechtern eine verminderte Wasseraufnahme festgestellt, die
Koerpergewichtsentwicklung war jedoch nicht signifikant beeinflusst. Klinische Veraenderungen waren Ataxie, Lethargie, bei einigen Tieren wurde gestraeubtes Fell, Dyspnoe, Hypothermie und Bewusstlosigkeit beschrieben. Keine Veraenderungen wurden bei klinisch-chemischen und haematologischen Untersuchungen festgestellt. Die absoluten Magen- und Lebergewichte waren erhoeht, die absoluten Hodengewichte verringert. Auch die relativen Magen- und Lebergewichte waren erhoeht, wie auch die relativen Milzgewichte bei den weiblichen Tieren. Bei den maennlichen Tieren waren die relativen Hodengewichte verringert. Bei den ueberlebenen Tieren dieser Dosisgruppe wurden Laesionen im Vormagen beschrieben.
2 Tiere der 1000 mg/kg Dosisgruppe starben waehrend der Versuchsdauer. Bei 6 maennlichen und 3 weiblichen Tieren der 1000 mg/kg Dosisgruppe wurden klinischen Veraenderungen

festgestellt,
diese entsprachen denen in der hoechsten Dosisgruppe.
Veraenderte Organgewichte und Laesionen des Vormagens wurden auch in dieser Dosisgruppe festgestellt.
Bei den Tieren der 330 mg/kg Dosisgruppe wurden keine klinischen Veraenderungen festgestellt. Bei den Tieren wurden jedoch z.T. erhoehte Magen- und Lebergewichte festgestellt, auch zeigten die Tiere Laesionen im Vormagen.
In der 100 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.

Source: BASF AG Ludwigshafen

(123)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 11 Tage
Frequency of treatment: einmal taeglich, 5 Tage / Woche
Post. obs. period: keine
Doses: 100; 330; 1000; 1500 mg/kg in waessriger Emulsion appliziert
Control Group: yes, concurrent vehicle
NOAEL: 100 - 330 mg/kg
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Je 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert dem 5 ul/100 ml Cremophor EL zugesetzt wurden.
4 weibliche und 1 maennliches Tier der 1500 mg/kg Dosisgruppe, ein weibliches Tier der 1000 mg/kg Dosisgruppe und ein maennliches Tier der Kontrollgruppe starben waehrend der Versuchsdauer.
In der 1500 mg/kg Dosisgruppe wurde kein Effekt auf die Koerpergewichtsentwicklung festgestellt. Klinische Veraenderungen waren Ataxie, Lethargie, bei einigen Tieren gestraeubtes Fell und Bewusstlosigkeit. Klinisch-chemische und haematologische Untersuchungen zeigten keine Veraenderungen. Absolute und relative Leber- und Magengewichte waren erhoeht. Bei den meisten Tieren wurden Foci im Vormagen beschrieben. Histologisch wurde im Vormagen der Tiere Hyperkeratose, Akanthose (fokal, multifokal) und entzuendliche Oedeme der Submucosa beschrieben, bei einigen Tieren auch Ulcerationen der Schleimhaut. In der Leber wurde eine Hypertrophie der Hepatocyten, bei 2 Tieren fokale Nekrosen der Leberzellen beschrieben. Bei 2 maennlichen Tieren wurden tubulaere Riesenzellen bilateral in den testikulaeren Tubuli beobachtet. Tubulaere Dilatationen und Nephrosen der Nierenrinde wurden bei den Tieren, die waehrend des Versuchs starben festgestellt, bei einem Tier wurden auf centrilobulaer fettige Infiltrationen in der Leber festgestellt.
Auch in der 1000 mg/kg Dosisgruppe traten die Befunde der hoechsten Dosierung bei einigen Tieren auf.
In der 330 mg/kg Dosisgruppe wurden bei einem Tier klinische

Veraenderungen (Ataxie, gestraeubtes Fell) beschrieben, auch wurden histologisch bei einigen Tieren im Vormagen Akanthose und Hyperkeratose der Schleimhaut festgestellt.
In der 100 mg/kg Dosisgruppe wurden keine substanzbedingten Effekte festgestellt.

Source: BASF AG Ludwigshafen

(124)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 3 Monate
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 25; 125; 250; 500 mg/kg
Control Group: yes, concurrent vehicle
NOAEL: 125 - 250 mg/kg
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Es wurden je 10 maennliche und 10 weibliche Tiere in die Versuchs- und Kontrollgruppen eingesetzt. Die Substanz wurde in 10 ml/kg Wasser appliziert, dem 5 ul/100 ml Cremophor EL zugesetzt waren. Ein Tier der 250 mg/kg Dosisgruppe starb waehrend der Versuchsdauer.
In der 500 mg/kg Dosisgruppe wurden keine substanzbedingten klinischen, klinisch-chemischen und haematologischen Veraenderungen festgestellt. Das relative Magengewicht der maennlichen Tiere war erhoeht. Bei 2 maennlichen und einem weiblichen Tier wurde geringgradig Akanthose (fokal und multifokal) in der Mucosa des Vormagens beschrieben.
In der 250 mg/kg Dosisgruppe wurde als einziger substanzbedingter Effekt ein erhoehtes relatives Magengewicht bei den maennlichen Tieren festgestellt.
In der 25 und 125 mg/kg Dosisgruppe wurden keine Veraenderungen festgestellt.

Es wurde zusaetzliche eine Satellitenstudie mit je 3 maennlichen und weiblichen Tieren pro Dosis- und Kontrollgruppe durchgefuehrt. Bei diesen Tieren wurde am Ende der Studie das Leber- und Knochenmarkgewebe fuer elektronenmikroskopische Untersuchungen praepariert. Es wurden keine substanzbedingten Effekte festgestellt. Keine Induktion der Cyanid-resistenten Palmitoyl-CoA-Oxidase wurde festgestellt.

Source: BASF AG Ludwigshafen

(125) (126)

Species: **Sex:**
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Post. obs. period:
Doses:
Control Group:
Method:
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: up to 5000 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: according to Ames BN et al, Mutat Res 31, 347-364 (1975)
Year: 1975 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(127)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration: 10, 33, 100, 220 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: according to Ames BN, et al. Mut Res 31, 347-364, 1975
Year: 1975 **GLP:** no data
Test substance: other TS: Purity 99%
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(128)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 0.01, 0.05, 0.25, 0.50, 1.0 ul/plate
Metabolic activation: with and without
Result: negative
Method: other: according to Ames BN, et al. Mut Res 31, 347-364, 1975.
Year: 1975 **GLP:** yes
Test substance: no data
Remark: Solvent:DMSO
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(129)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 0.002-1.8 ul/plate
Metabolic activation: with and without
Result: negative
Method: other: according to Ames BN,et al. Mut Res 31, 347-364 (1975)
Year: 1975 **GLP:** yes
Test substance: no data
Remark: Solvent: DMF
2-Ethylhexanol was tested at dose levels of 0.002 to 1.8 ul/plate. In a separate toxicity test using the TA 100 strain, 80% toxicity was observed at 1.8 ug/plate in the

absence of metabolic activation. The treatment did not induce statistically significant increases in the frequency of His+ revertants.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(130)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 10, 100, 500, 1000, 5000 ug/plate
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** yes
Test substance: no data
Remark: Solvent: ethanol.
2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all tester strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or wothout activation.
Source: Neste Oxo AB Stenungsund

(131)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 4 to 2800 ug/plate
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** no data
Test substance: other TS: purity >97%
Remark: 2-Ethylhexanol was tested in the standard plate incorporation assay. Toxicity was observed in all tester strains at 2800 ug/plate.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(132)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538, TA 2637
Concentration: 500 ug/plate
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(133)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 1, 5, 10, 50, 100, 500, 1000 ug/plate
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:**
Test substance: other TS: 2-EH 98%
Remark: Solvent: DMSO
The preincubation method was used. Except for TA 1537 toxicity was observed at doses of 500 and 1000 ug/plate in all tester strains.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(134)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration:
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** no data
Test substance: other TS: purity >97%
Remark: The mutagenicity of urin from Sprague-Dawley rats dosed daily by gavage for 15 days with 2,000 mg/kg of 2-ethylhexanol was evaluated. Cultures were dosed with up to 2 ml urine using direct plating procedures.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(135)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 10, 100, 500, 1000, 5000 ug/plate
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** yes
Test substance: no data
Remark: Solvent: ethanol.
2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all tester strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or wothout activation.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(136)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 10, 100, 500, 1000, 5000 ug/plate
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** yes
Test substance: no data
Remark: Solvent: ethanol.
2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all tester strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or wothout activation.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(136)

Type: Bacterial gene mutation assay
System of testing: Salmonella typhimurium TA 100
Concentration: 0.5, 1.0, 1.5 mM
Metabolic activation: with and without
Result: positive
Method: other: as described by author
Year: 1982 **GLP:** no data
Test substance: no data
Remark: The mutagenic activity of 2-ethylhexanol was evaluated in an 8-azaguanine resistance assay. 2-ethylhexanolwas noted to be weakly mutagenic in a dose dependent way.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(137)

Type: Bacterial gene mutation assay
System of testing: Bacillus subtilis H17/M45
Concentration: 500 ug/plate
Metabolic activation:
Result: negative
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(138)

Type: Cytogenetic assay
System of testing: Chinese hamster ovary (CHO) cells
Concentration: 1.5-2.8 mM
Metabolic activation:
Result: ambiguous
Method:
Year: **GLP:**
Test substance:
Remark: At 2.4 mM 2-ethylhexanol had a very slight effect on chromosomal integrity.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(139)

Type: DNA damage and repair assay
System of testing: E. coli strain W3110 (pol A+) and p3478 (pol A-)
Concentration: 10, 50, 100, 250, 500 ug/ml
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** yes
Test substance: other TS: purity 99.7%
Remark: 2-Ethylhexanol was examined for DNA modifying activity in E. coli strain W3110 (pol A+) and its polymerase deficient derivative p3478 (pol A-). Based on a range finding study, the test article, dissolved in ethanol, was administered to cells at concentrations of 10, 50, 100, 250 and 500 ug/ml of

bacterial suspension. Results were equivocal, however, as the test vehicle, ethanol, was found to be positive in the assay. The experiment was repeated using DMSO as the test vehicle and results were negative for 2-ethylhexanol.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(136)

Type: HGPRT assay
System of testing: CHO cells
Concentration: 20-400 nl/ml
Metabolic activation: with and without
Result: negative
Method: other: as described by author
Year: 1985 **GLP:** yes
Test substance: no data
Remark: 2-Ethylhexanol was tested at concentrations of 20 to 300 nl/ml in the absence, and 100 to 400 nl/ml in the presence of Arochlor-induced rat liver S9 fraction. Reproducible increases in mutant frequencies of CHO-cells were not observed.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(140)

Type: Mouse lymphoma assay
System of testing: L5178Y TK+/- mouse lymphoma cells
Concentration: 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18,.0.24 ul/ml
Metabolic activation: with and without
Result: negative
Method: other: as described by author
Year: 1983 **GLP:** yes
Test substance: other TS: purity >99.7%
Source: Neste Oxo AB Stenungsund

(141)

Type: Mouse lymphoma assay
System of testing: L5178Y TK+/- mouse lymphoma cells
Concentration: 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18,.0.24 ul/ml
Metabolic activation: with and without
Result: negative
Method: other: as described by author
Year: 1983 **GLP:** yes
Test substance: other TS: purity >99.7%
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(129)

Type: Mouse lymphoma assay
System of testing: L5178Y TK+/- mouse lymphoma cells
Concentration: 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18,.0.24 ul/ml
Metabolic activation: with and without
Result: negative
Method: other: as described by author
Year: 1983 **GLP:** yes
Test substance: other TS: purity >99.7%
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(129)

Type: Unscheduled DNA synthesis
System of testing: Primary rat hepatocytes
Concentration: 2.5, 5, 10, 25, 50, 100, 250, 500 and 1000 nl/ml
Metabolic activation: without
Result: negative
Method:
Year: **GLP:** yes
Test substance: other TS: purity > 99.7%
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(142)

Type: other: Cell transformation assay
System of testing: Balb/3T3 cells
Concentration: 0.011 to 1.5.ul/ml
Metabolic activation: without
Result: negative
Method: other: as described by author
Year: 1982 **GLP:** yes
Test substance:
Remark: 2-Ethylhexanol was tested in the cell transformation assay in Balb/C-3T3 mouse embryo cells exposed to concentrations of 1.5, 1.125, 0.75, 0.375, or 0.188 ul/ml under open vessel conditions, and 0.162, 0.129, 0.043 or 0.011 ul/ml under closed vessel conditions. No statistically significant increase in transformation rates was observed at any concentration.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(143)

Type: other: Cell transformation assay
System of testing: Balb/3T3 cells
Concentration: 0.011 to 1.5.ul/ml
Metabolic activation: without
Result: negative
Method: other: as described by author
Year: 1982 **GLP:** yes
Test substance:
Remark: 2-Ethylhexanol was tested in the cell transformation assay in Balb/C-3T3 mouse embryo cells exposed to concentrations of 1.5, 1.125, 0.75, 0.375, or 0.188 ul/ml under open vessel conditions, and 0.162, 0.129, 0.043 or 0.011 ul/ml under closed vessel conditions. No statistically significant increase in transformation rates was observed at any concentration.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(130)

Type: other: Cell transformation assay
System of testing: Mouse JB6 C141 cells
Concentration: 0.4 - 7.7 umol/l
Metabolic activation: without
Result: negative
Method: other: see reference
Year: 1986 **GLP:** no data
Test substance: no data
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(144)

Type: other: Cell transformation assay
System of testing: Balb/3T3 Clone A31 mouse embryo cells
Concentration: 30, 100 and 300 nl/ml
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** yes
Test substance: other TS: purity > 99.7%
Source: Neste Oxo AB Stenungsund

(131)

Type: other: Cell transformation assay
System of testing: Balb/3T3 Clone A31 mouse embryo cells
Concentration: 30, 100 and 300 nl/ml
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** yes
Test substance: other TS: purity > 99.7%
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(136)

Type: other: Cell transformation assay
System of testing: Balb/3T3 Clone A31 mouse embryo cells
Concentration: 30, 100 and 300 nl/ml
Metabolic activation: with and without
Result: negative
Method:
Year: **GLP:** yes
Test substance: other TS: purity > 99.7%
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(136)

Type:
System of testing:
Concentration:
Metabolic activation:
Result:
Method:
Year: **GLP:**
Test substance:
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5.6 Genetic Toxicity 'in Vivo'

Type: Cytogenetic assay
Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 5 days
Doses: 0.02, 0.07, 0.21 ml/kg day
Result:
Method: other: as described by author
Year: 1981 **GLP:** yes
Test substance: other TS: purity > 99.7%
Result: Result: Groups of 5 male F-344 rats were treated with 2-ethylhexanol. Of the 50 metaphase bone marrow cells examined from each animal, no significant increase in chromatid and chromosome breaks or structural rearrangements was noted. In addition, the mitotic index was unaffected by 2-ethylhexanol. At the dose levels tested 2-ethylhexanol did not induce detectable chromosomal aberrations after oral administration.
Source: Neste Oxo AB Stenungsund

Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(145)

Type: Dominant lethal assay
Species: mouse **Sex:** male
Strain: ICR
Route of admin.: oral unspecified
Exposure period: 5 days
Doses: 250, 500 and 1000 mg/kg
Result:
Method: other: as described by author
Year: 1981 **GLP:** yes
Test substance: other TS: purity 99.7%
Result: After treatment, each male was housed with 2 virgin females per week for 8 consecutive weeks to span the spermatogenic cycle. Females were sacrificed on day 14-17 of caging and scored for pregnancy, living fetuses and early and late fetal deaths. The fertility indicies and the average number of dead and total implants per pregnancy were within the normal range. It was concluded that 2-ethylhexanol did not induce dominant lethal mutations after oral administration.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(146)

Type: Drosophila SLRL test
Species: Drosophila melanogaster **Sex:** male
Strain:
Route of admin.: other: injection
Exposure period: single application
Doses: 50000 ppm
Result:
Method: other: as described by author
Year: 1985 **GLP:** no data
Test substance: other TS: Purity>99%
Result: 2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.
Source: Neste Oxo AB Stenungsund

(147)

Type: Drosophila SLRL test
Species: Drosophila melanogaster **Sex:** male
Strain:
Route of admin.: oral feed
Exposure period: 72 hours
Doses: 20000 ppm
Result:
Method: other: as described by author
Year: 1985 **GLP:** no data
Test substance: other TS: 2-EH 99%
Result: Male flies were fed 2-ethylhexanol in a solution of 5% aqueous sucrose. The test substance was not mutagenic by this route.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(148)

Type: Drosophila SLRL test
Species: Drosophila melanogaster **Sex:** male
Strain:
Route of admin.: other: injection
Exposure period: single application
Doses: 50000 ppm
Result:
Method: other: as described by author
Year: 1985 **GLP:** no data
Test substance: other TS: Purity>99%
Result: 2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(148)

Type: Drosophila SLRL test
Species: Drosophila melanogaster **Sex:** male
Strain:
Route of admin.: other: injection
Exposure period: single application
Doses: 50000 ppm
Result:
Method: other: as described by author
Year: 1985 **GLP:** no data
Test substance: other TS: Purity>99%
Result: 2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(148)

Type: Micronucleus assay
Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: i.p.
Exposure period: single administration
Doses: 456 mg/kg
Result:
Method: other: as described by author
Year: 1982 **GLP:** yes
Test substance: no data
Result: B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.
Source: Neste Oxo AB Stenungsund

(149)

Type: Micronucleus assay
Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: i.p.
Exposure period: single administration
Doses: 456 mg/kg
Result:
Method: other: as described by author
Year: 1982 **GLP:** yes
Test substance: no data
Result: B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(150)

Type: Micronucleus assay
Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: i.p.
Exposure period: single administration
Doses: 456 mg/kg
Result:
Method: other: as described by author
Year: 1982 **GLP:** yes
Test substance: no data
Result: B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.
Source: Neste Oxo AB Stenungsund

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(150)

Type: Micronucleus assay
Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: i.p.
Exposure period: two administrations
Doses: 456 mg/kg
Result:
Method:
Year: **GLP:**
Test substance:
Result: B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 24 hrs after the second administation (the two administrations being 24 hrs apart) and 1000 PCE/animal were scored for the presence of micronuclei. 2-ethylhexanol was not considered to be clastogenic under the conditions of this assay.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(150)

5.7 Carcinogenicity

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 24 months
Frequency of treatment: 5 days/week
Post. obs. period: none
Doses: 0, 50, 150, 500 mg/kg
Result:
Control Group: yes, concurrent vehicle
Method: other: according to EPA-TSCA guidelines
Year: **GLP:** yes
Test substance: other TS: purity 99.8%
Remark: Vehicle: aqueous 0.005% Cremophor EL.
In addition to the vehicle control groups, 50 rats/sex were dosed with water;
Concurrently to the main study, a satellite study was performed. 2-Ethylhexanol was administered by gavage (same vehicle as in the main study) at a dose of 500 mg/kg. One group of rats (10/sex; interim sacrifice group) was treated with 2-ethylhexanol 5 days/week over a period of 18 months

and then sacrificed. Another group (50 rats/sex; recovery group) was treated with the same dose for 18 months and thereafter with vehicle only for 6 months and then sacrificed. As a control group for the interim sacrifice group 10 male and 10 female rats received the vehicle for 18 months. Control data for the recovery group were adopted from the vehicle control group and the top dose group of the parallel main study.

Result: Result:

Satellite study:

In the interim sacrifice group a reduced body weight gain (both sexes) and clinical symptoms like poor general condition, labored breathing and "genital region smeared with urine" (females only) was observed. A slightly increased mortality in females was observed. The relative weight of testes and brain (males), stomach (females), liver and kidney (both sexes) were increased. In the recovery group similar effects were observed. After termination of treatment the body weight gain increased indicating a recovery effect. 18 males and 17 females died prematurely and one each had a focal hyperplasia in the forestomach. In the glandular stomach erosions were seen in 4 males and females each. Glandular cysts occurred in 6 males and 8 females.

Main study:

2-Ethylhexanol was not oncogenic in the rat under the conditions of this assay. In both sexes the sum of primary tumors, the sum of benign tumors and the sum of malignant tumors was lower in the top dose group than in either the vehicle control or the water control groups.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(151)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 24 Monate
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 50; 150; 500 mg/kg
Result:
Control Group: yes, concurrent vehicle
Method: other: EPA - TSCA oncogenicity guidelines, 798.3300
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Es wurden je 50 maennliche und 50 weibliche Tiere in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert, dem 5 mg/100 ml Cremophor EL zugesetzt waren.
In der 50 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.
150 mg/kg bewirkten eine Reduktion der Koerpergewichtsentwicklung bei den maennlichen Tieren um 16 % bei den weiblichen um 12 %. Es wurde eine leichte Zunahme der Anzahl von Tieren mit klinischen Veraenderungen (schlechter Allgemeinzustand, erschwerte Atmung, gestraeubtes Fell, Urin auf dem Fell im Genitalbereich) beschrieben.
Bei den Tieren der 500 mg/kg Dosisgruppe wurde eine starke Reduktion der Koerpergewichtsentwicklung festgestellt (31 - 33 %). Bei den weiblichen Tieren war die Mortalitaetsrate signifikant erhoeht (58 % gegenueber 28 % in der Kontrollgruppe). Die Zahl der Tiere mit klinischen Veraenderungen war erhoeht. Bei haemotologischen Untersuchungen wurde nach 12 Monaten Behandlungsdauer bei den maennlichen Tieren eine leichte Zunahme von Anisocytose, vorwiegend Microcytose, beschrieben. Dieser Befund wurde nach 18 und 24 Monaten nicht mehr festgestellt. Pathologisch wurde bei den Tieren eine Ansteigen der Bronchopneumonien beschrieben, das in Verbindung mit der Aspiration von Mageninhalten gesehen wurde. Es wurde keine erhoehte Tumorinzidenz festgestellt, die Summe der Tumoren war geringer als in der Kontrollgruppe.
Zur Hauptstudie wurde zusaetzlich eine Satellitenstudie mit der hoechsten Dosierung, 500 mg/kg durchgefuehrt. 2 Versuchsgruppen wurden eingesetzt, in der ersten Versuchsgruppe (10 maennliche und 10 weibliche Tiere) wurden die Tiere nach 18 Monaten getoetet und untersucht. In der 2 Versuchsgruppe (50 maennliche und 50 weibliche Tiere) wurden die Tiere 18 Monate mit der Substanz behandelt, danach 6 Monate entsprechend der Kontrolle.
Die Futteraufnahme war bei den maennlichen Tieren, die nach 18 Monaten getoetet wurden reduziert, die Koerpergewichtsentwicklung war bei den maennlichen Tieren um 28 % bei den weiblichen um 14 % reduziert. Eine Zunahme der Tiere mit schlechtem Allgemeinzustand wurde beschrieben, die Mortalitaet der weiblichen Tiere war erhoeht. Veraenderte Organgewichte wurden beschrieben.

Bei den Tieren, die nach 18 Monaten Behandlung eine 6-monatige Recovery-Phase hatte wurden folgende Veraenderungen beschrieben: reduzierte Futteraufnahme bei den maennlichen Tieren, die waehrend der Behandlung stark reduzierte Koerpergewichtsentwicklung war nach der Recovery-Phase weniger stark ausgepraegt. Klinischen Veraenderungen (schlechter Allgemeinzustand, erschwerte Atmung, Urin auf dem Fell in Genitalbereich) wurden festgestellt, auch die Organgewichte waren veraendert. Die Autoren sehen nur einen leichten Erholungseffekt waehrend der Recovery-Phase, aufgrund der Koerpergewichtsentwicklung.

Source: BASF AG Ludwigshafen

(152) (153)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 18 months
Frequency of treatment: 5 days/week
Post. obs. period: none
Doses: 0, 50, 200, 750 mg/kg
Result:
Control Group: yes, concurrent vehicle
Method: other: according to EPA-TSCA guidelines
Year: **GLP:** yes
Test substance: other TS: purity 99.8%
Remark: Vehicle: aqueous 0.005% Cremophor EL
In addition to the vehicle control groups, 50 mice/sex were dosed with water.
Concurrently to the main study, a satellite study was performed: 2-Ethylhexanol was administered by gavage (same vehicle as in the main study) at a dose of 750 mg/kg. One group of mice (10/sex; interim sacrifice group) was treated with 2-ethylhexanol 5 days/week over a period of 13 months and then sacrificed. Another group (50 mice/sex; recovery group) was treated with the same dose for 13 months and thereafter with vehicle only for 5 months and then sacrificed. As a control group for the interim sacrifice group 10 male and 10 female mice received the vehicle for 13 months. Control data for the recovery group were adopted from the vehicle control group and the top dose group of the parallel main study.

Result: Result:

Satellite study:

The administration of 2-ethylhexanol to male and female mice for 13 months at a dose of 750 mg/kg caused increased mortality, reduced feed consumption and body weight gain in both sexes. The body weight gain of male and female animals of the recovery group were reduced as long as the animals were treated. After termination of treatment the male animals gained weight and reached nearly the values of the control group, indicating a recovery effect. No such effect was seen in females.

Pathology revealed some statistically significant changes in organ weights and masses of foci in liver and stomach. One male and one female animal of the recovery group which died premarurely had a focal hyperplasia in the forestomach.

Main study:

2-Ethylhexanol was not oncogenic in the mouse under the conditions of this assay. A slight increase in the incidence of hepatocellular carcinoma in the females of the high dose group was statistically significant if compared to the control group dosed with the emulsion vehicle, but not when compared to the control group dosed with water. This difference was regarded as incidental and not biologically relevant, based upon comparison with published data, and because of the lack of metastases. No statistically significant increase in tumor incidence occured in male mice.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(154)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 18 Monate
Frequency of treatment: einmal taeglich, 5 Tage/Woche
Post. obs. period: keine
Doses: 50; 200; 750 mg/kg
Result:
Control Group: yes, concurrent vehicle
Method: other: EPA-TSCA oncogenicity guidelines (798.3300)
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Je 50 maennliche und 50 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser, dem 5 mg/100 ml Cremophor EL zugesetzt waren, appliziert.
In der 50 und 200 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.
In der 750 mg/kg Dosisgruppe war die Koerpergewichtsentwicklung bei den maennlichen Tieren um 26 % bei den weiblichen um 24 % reduziert, verbunden mit einer reduzierten Futteraufnahme. Die Mortalitaet war signifikant erhoeht (30 % bei beiden Geschlechtern gegenueber 4 % bei maennlichen und 8 % bei weiblichen Kontrolltieren). Bei haematologischen Untersuchungen wurde ein leichter Anstieg der polymorphkernigen Neutrophilen und eine Verminderung der

Leukocyten festgestellt.
Im Vormagen der Tiere wurde eine Zunahme der fokalen Hyperplasien des Epithels beobachtet. Bei den weiblichen Tieren wurde ein leichter Anstieg der hepatocellulaeren Carcinome festgestellt, der im Vergleich zur Kontrolle signifikant war. Im Vergleich zu historischen Kontrollen war das vermehrte Auftreten von hepatocellaeren Carcinomen jedoch nicht signifikant, es wurden auch keine Metastasen festgestellt. Die Autoren beurteilen die Inzidenz der beobachteten Tumoren als zufaellig und ohne biologische Relevanz.
Zur Hauptstudie wurde zusaetzliche eine Satellitenstudie durchgefuehrt. Die Tiere in der Satellitenstudie erhielten nur die hoechste Dosierung, d.h. 750 mg/kg. In der Satellitenstudie waren 3 Gruppen: eine Kontrollgruppe mit je 10 maennlichen und 10 weiblichen Tieren, eine Versuchsgruppe mit 10 weiblichen und 10 maennlichen Tieren, die Tiere dieser Gruppe wurden nach 13 Monaten Behandlung getoetet und eine weitere Versuchsgruppe mit je 50 maennlichen und 50 weiblichen Tieren, die 13 Monate behandelt wurden und danach bis zum Versuchsende (18 Monate) entsprechend der Kontrolle behandelt wurden.
Veraenderungen bis zur Interimstoetung nach 13 Monaten waren: erhoehte Mortalitaet, reduzierte Futteraufnahme und reduzierte Koerpergewichtsentwicklung.
In der Versuchsgruppe, in der die Tiere nach 13 Monaten Substanzbehandlung noch 5 Monate beobachtete wurden, zeigten die maennlichen Tiere nach Absetzen der Behandlung eine deutliche Zunahme der Koerpergewichtsentwicklung, so dass nach 18 Monaten kein signifikanter Unterschied zu den Kontrollen festzustellen war. Bei den weiblichen Tieren wurde dieser Effekt nicht festgestellt.
Bei pathologischen Untersuchungen der behandelten Tiere wurden signifikante Unterschiede bei Organgewichten festgestellt, wie auch Focibildung in der Leber und im Magen.

Source: BASF AG Ludwigshafen

(155) (156)

5.8 Toxicity to Reproduction

Type:
Species: **Sex:**
Strain:
Route of admin.:
Exposure Period:
Frequency of treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: **GLP:**
Test substance:
Remark: No study located.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5.9 Developmental Toxicity/Teratogenicity

Species: rat **Sex:** female
Strain: Sprague-Dawley
Route of admin.: inhalation
Exposure period: gestation day 1 to 19
Frequency of treatment: daily (7 hours)
Duration of test: 20 days
Doses: 850 mg/m3
Control Group: yes
Method: other: as described by author
Year: 1989 **GLP:** no data
Test substance: other TS: purity >99%
Result: Result: A group of Sprague-Dawley rats was exposed for 7 hours per day on gestation days 1-19 to 2-ethylhexanol at hte highest concentration that could be generated as a vapour. Dams were sacrificed on day 20. 2-Ethylhexanol reduced maternal feed intake, but did not produce any malformations.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(157)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: gavage
Exposure period: gestation day 6 through 15
Frequency of treatment: daily
Duration of test: 20 days
Doses: 130, 650, 1300 mg/kg day (in bidist. water containing 0.005% Cremophor EL)
Control Group: yes, concurrent vehicle
NOAEL Maternalt.: = 130 mg/kg bw
NOAEL Teratogen.: = 650 mg/kg bw
Method: Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year: 1987 **GLP:** yes
Test substance: other TS: purity >99.5%
Result: Results:

2-Ethylhexanol was tested in this screening study (10 animals per dose group) for its prenatal toxicity in Wistar rats. On day 20 post coitum all surviving animals were sacrificed and assessed by gross pathology. The fetuses were dissected from the uterus, sexed, weighed and further investigated for any external, soft tissue and/or skeletal findings.

130 mg/kg dose group:
No adverse substance-related effects on dams of fetuses.

650 mg/kg dose group:
* maternal toxic effects
- 2 dams with piloerection
* embryo/fetotoxic effects
- slightly reduced mean fetal body weights
- increased frequency of fetuses with skeletal variations and retardations

1300 mg/kg dose group:
* maternal toxic effects
- markedly reduced food consumption during the whole treatment period (days 6-15 p.c.)
- distinctly reduced mean body weights (day 10 -20 p.c.) body weight loss during days 6-10 p.c. and reduced body body weight gains during days 10-15 p.c.; markedly reduced corrected body weight gain
- 6 animals found dead on days 9, 10 and 13 p.c.
- severe clinical sypmtoms like abdominal or lateral position, unsteady gait and apathy
- light brown-gray discoloration of the liver in the animals with intercurrent death; lund edema and emphysema in a few animals, and hemometra in 1 dam which showed vaginal hemorrage before death
- distinctly reduced mean uterus weight
* embryo/fetotoxic effects
- increased number of resorptions and consequently markedly increased postimplantation loss
- markedly reduced mean fetal body weights

- one fetus with acaudia and atresia ani; increased incidence of fetuses with dilated renal pelvis and/or hydroureter higher number of fetuses with skeletal malformations, variations and retardations.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(158)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: gavage
Exposure period: single application on day 12 of gestation
Frequency of treatment: single application on day 12 of gestation
Duration of test:
Doses: 6.25, 12.5 mmol/kg (833, 1666 mg/kg)
Control Group: yes, concurrent no treatment
Method: other: as described by author
Year: 1985 **GLP:** no data
Test substance: no data
Result: Results: The group given 833 mg/kg showed a slight increase of 2% in malformed fetuses relative to the controls (0%). The other parameters (implantation index, mean fetal weight, number of dead and resorbed fetuses) were unaffected. Simultaneous intraperitoneal administration of 150 mg caffeine / kg potentiated this effect (increase in malformed fetuses to 21.2 %). Even after a dose of 1666 mg/kg, the implantation index and percentage of dead and resorbed fetuses were unchanged, although the mean fetal body weight at 3.5 g was reduced relative to the controls (4.1 g). 22.2 % of the surviving fetuses showed malformations (controls 0%). These included hydronephrosis (7.8%), tail anomalies (4.9%), anomalies of the extremities (9.7%) and "others" (1%).

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(159)

- one fetus with acaudia and atresia ani; increased incidence of fetuses with dilated renal pelvis and/or hydroureter higher number of fetuses with skeletal malformations, variations and retardations.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(158)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: gavage
Exposure period: single application on day 12 of gestation
Frequency of treatment: single application on day 12 of gestation
Duration of test:
Doses: 6.25, 12.5 mmol/kg (833, 1666 mg/kg)
Control Group: yes, concurrent no treatment
Method: other: as described by author
Year: 1985 **GLP:** no data
Test substance: no data
Result: Results: The group given 833 mg/kg showed a slight increase of 2% in malformed fetuses relative to the controls (0%). The other parameters (implantation index, mean fetal weight, number of dead and resorbed fetuses) were unaffected. Simultaneous intraperitoneal administration of 150 mg caffeine / kg potentiated this effect (increase in malformed fetuses to 21.2 %). Even after a dose of 1666 mg/kg, the implantation index and percentage of dead and resorbed fetuses were unchanged, although the mean fetal body weight at 3.5 g was reduced relative to the controls (4.1 g). 22.2 % of the surviving fetuses showed malformations (controls 0%). These included hydronephrosis (7.8%), tail anomalies (4.9%), anomalies of the extremities (9.7%) and "others" (1%).

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(159)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: gavage
Exposure period: 6.- 15. Tag der Traechtigkeit
Frequency of treatment: einmal taeglich
Duration of test: bis zum 20. Tag der Traechtigkeit
Doses: 130; 650; 1300 mg/kg
Control Group: yes
Method: other
Year: **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Result: Je 10 Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 5 ml/kg bidest. Wasser appliziert, das zu 0.005 % Cremophor EL enthielt.

Die niedrigste Dosierung hatte keine Wirkung auf die Muttertiere und Feten.

650 mg/kg fuehrten bei 2 Muttertieren zu gestraeubtem Fell. Das Fetengewicht war leicht reduziert und die Zahl der skelettalen Variationen und Retardierungen erhoeht.

1300 mg/kg bewirkten deutliche maternale Toxizitaet. 6 Muttertiere starben waehrend der Versuchsdauer. Die maternale Futteraufnahme war waehrend der Behandlungsdauer deutlich reduziert. Sowohl die Koerpergewichtsentwicklung wie auch das Koerpergewicht zu Versuchsende waren reduziert. Deutliche klinische Symptome traten auf. Bei den Tieren die waehrend der Behandlungsdauer starben wurden braun-graue Verfaerbungen der Leber beschrieben, Lungenoedeme und -emphyseme. Das Uterusgewicht war deutlich reduziert. Die Zahl der Resorptionen und Postimplantationsverluste war deutlich erhoeht, die Fetengewichte reduziert. Bei einem Fetus wurde Schwanzlosigkeit und Analatresie festgestellt. Die Zahl der Feten mit erweiterten Nierenbecken und Hydroureter war erhoeht, wie auch die Zahl der Feten mit skelettalen Missbildungen, Variationen und Retardierungen.
Source: BASF AG Ludwigshafen

(160)

Species: mouse **Sex:** female
Strain: CD-1
Route of admin.: gavage
Exposure period: gestation day 7 through 14
Frequency of treatment: daily
Duration of test:
Doses: 1525 mg/kg
Control Group: yes, concurrent vehicle
Method: Chernoff-Kavlok teratogenicity screening test
Year: 1980 **GLP:** yes
Test substance: no data
Remark: Vehicle : corn oil.

Observation period: until day 3 post partum.

The results of this study regarding the influence of 2-ethylhexanol on reproduction should be taken with care since the dose applied resulted in the death of more than 30 % of treated dams. Therefore, the observed effects on the offspring should be attributed to the extensive maternal toxicity and are very unlikely to be primary effects. The authors state that the results of this assay should not be used to label a chemical as teratogenic or nonteratogenic but to establish priorities for conventional testing.

Result: This screening test was conducted with one group of 50 pregnant CD-1 mice. The dose of 1525 mg 2-ethylhexanol/kg/day was determined previously as the minimal effective dose for adult female mice. In 17 animals, test substance related mortality was observed by the end of the treatment period. Another animal died because of a dosing error. Clinical observations in dams included languidity, ataxia, coldness to touch, wet stains, oily coat, and dark red discharge from the anus of one animal. Decreases in body weights and the reproductive index were observed in treated animals compared to controls. Decreases were also observed in the following parameters when compared to controls: mean number of live pups per litter, litter weight, pup weight on days 1 and 3, percent change in pup weight from day 1 to day 3, mean pup viability per litter from day 1 to 3, and percent of live pups per litter on day 1 post partum. The mean number and percent of dead pups in the treatment group was reported to be greater than in the control group.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(161)

Species: mouse **Sex:** female
Strain: CD-1
Route of admin.: oral feed
Exposure period: gestation day 0 through 17
Frequency of treatment: daily (microencapsulated in the diet)
Duration of test:
Doses: 0, 17, 59, 191 mg/kg/day
Control Group: yes
NOAEL Maternalt.: > 191 mg/kg bw
NOAEL Teratogen.: > 191 mg/kg bw
Method: other: as described by author
Year: 1991 **GLP:** yes
Test substance: other TS: purity >99%
Result: Result: No dams died, delivered early or were removed from the study. Pregnancy rate was high and equivalent across all groups. There was no treatment-related maternal toxicity observed in this study.

There were no effects of exposure to diatary 2-ethylhexanol on any gestational parameters. The number of corpora lutea, uterine implantation sites, pre- and postimplantation loss, sex ratio and live fetal body weight per litter were all equivalent across all groups. There were also no treatment-related changes in the incidence of individual, external, visceral, skeletal or total malformations or variations. In conclusion, there were no maternal or developmental toxic effects of 2-ethylhexanol dietary exposure throughout gestation at any concentration tested.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(162)

Species: rat **Sex:** female
Strain: Fischer 344
Route of admin.: dermal
Exposure period: gestation day 6 through 15
Frequency of treatment: daily (6 hours)
Duration of test: 21 days
Doses: 0.3, 1.0, 3.0 ml/kg/day (252, 840, 2520 mg/kg/day)
Control Group: yes
NOAEL Maternalt.: = 252 - 840 mg/kg bw
NOAEL Teratogen.: > 2520 mg/kg bw
Method: other: according to US EPA Health Effect Guidelines
Year: 1989 **GLP:** yes
Test substance: other TS: purity >99.7%
Result: Result: Administration of 2-ethylhexanol by occluded cutaneous application to time-pregnant Fischer 344 rats during organogenesis at 0, 0.3, 1.0, or 3.0 ml/kg/day (25 animals per dose) resulted in maternal toxicity at 1.0 and 3.0 ml/kg/day (clinical signs of toxicity at the dosing site for both doses and reduced weight gain in the treatment period at 3.0 ml/kg/day), and no developmental toxicity at any doses tested. There was no treatment-related increased incidence of malformations at any dosage employed.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(163)

5.10 Other Relevant Information

Type: adsorption
Remark: The percutaneous absorption rate of [14C]-2-ethylhexanol through human stratum corneum and full thickness rat skin has been measured in vitro using Franz-type glass diffusion cells. The absorption rate of 2-ethylhexanol through rat skin was 190 +-40 and 240 +-110 ug/cm2/hr in two separate studies. Similarly, the absorption rate through human stratum corneum was found to be 39 +-16 and 37 +- 10 ug/cm2/hr in two separate studies. The overall mean rate of percutaneous absorption through rat skin is 5.7 times the rate through human stratum corneum.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(164)

Type: adsorption
Remark: In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.
Source: Neste Oxo AB Stenungsund

(165)

Type: adsorption
Remark: In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(165)

Type: adsorption
Remark: In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(165)

Type: Biochemical or cellular interactions
Remark: The incubation of 325.6 to 1953.5 ug/ml 2-ethylhexanol with the 9000xg supernatant of rat liver homogenate dose dependently reduced the activities of the aniline hydroxylase and the aminopyrin-N-demethylase.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(166)

Type: Biochemical or cellular interactions
Remark: B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were pretrerated for 4 weeks with 1% di(2-ethylhexyl)-phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.
Source: Neste Oxo AB Stenungsund

(167)

Type: Biochemical or cellular interactions
Remark: The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawely rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.
Source: Neste Oxo AB Stenungsund

(168)

Type: Biochemical or cellular interactions
Remark: The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).
Source: Neste Oxo AB Stenungsund

(169)

Type: Biochemical or cellular interactions
Remark: Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the reminder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl -CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.
Source: Neste Oxo AB Stenungsund

(170)

Type: Biochemical or cellular interactions
Remark: Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.
Source: Neste Oxo AB Stenungsund

(171)

Type: Biochemical or cellular interactions
Remark: Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acteyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared to the control.
Source: Neste Oxo AB Stenungsund

(172)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.
Source: Neste Oxo AB Stenungsund

(173)

Type: Biochemical or cellular interactions
Remark: Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentraitons (3 nM), ethylhexanol also increased intracellular calcium.
Source: Neste Oxo AB Stenungsund

(174)

Type: Biochemical or cellular interactions
Remark: The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.

Source: Neste Oxo AB Stenungsund

(175)

Type: Biochemical or cellular interactions

Remark: Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O2/CO2-saturated buffer. Following infusion of ethylhexanol, O2 uptake and ketone body formation were diminished by 50 and 80%, respectilely, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O2-rich upstream regions of the liver lobule were damaged as reflected by trypan blue uptake. It is concluded, that the toxicity of ethylhexanol in the liver is dependent on local O2 tension and mitochondria are primary targets.

Source: Neste Oxo AB Stenungsund

(176)

Type: Biochemical or cellular interactions

Remark: 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration pereceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl2 by isolated mitochondria 4- to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.

Source: Neste Oxo AB Stenungsund

(177)

Type: Biochemical or cellular interactions

Remark: 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with 2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O2. The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.

Source: Neste Oxo AB Stenungsund

(178)

Type: Biochemical or cellular interactions
Remark: The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanolturned out to be weak.
Source: Neste Oxo AB Stenungsund

(179)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activitiy was detected.
Source: Neste Oxo AB Stenungsund

(180)

Type: Biochemical or cellular interactions
Remark: Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).
Source: Neste Oxo AB Stenungsund

(181)

Type: Biochemical or cellular interactions
Remark: Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-(2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.
Source: Neste Oxo AB Stenungsund

(100)

Type: Biochemical or cellular interactions
Remark: Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.
Source: Neste Oxo AB Stenungsund

(182)

Type: Biochemical or cellular interactions
Remark: The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a substancial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes, administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.
Source: Neste Oxo AB Stenungsund
(183)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.
Source: Neste Oxo AB Stenungsund
(184)

Type: Biochemical or cellular interactions
Remark: Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.
Source: Neste Oxo AB Stenungsund
(114)

Type: Biochemical or cellular interactions
Remark: The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.
Source: Neste Oxo AB Stenungsund
(185)

Type: Biochemical or cellular interactions
Remark: In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferaiton in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the immunochemical detectabel levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined. 2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).
Source: Neste Oxo AB Stenungsund

(186)

Type: Biochemical or cellular interactions
Remark: Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse heaptocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxsomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.
Source: Neste Oxo AB Stenungsund

(187)

Type: Biochemical or cellular interactions
Remark: B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were pretrerated for 4 weeks with 1% di(2-ethylhexyl)-phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(167)

Type: Biochemical or cellular interactions
Remark: The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawely rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(168)

Type: Biochemical or cellular interactions
Remark: The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(169)

Type: Biochemical or cellular interactions
Remark: Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the reminder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl -CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(170)

Type: Biochemical or cellular interactions
Remark: Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.
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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(171)

Type: Biochemical or cellular interactions
Remark: Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acteyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared to the control.
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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(172)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(173)

Type: Biochemical or cellular interactions
Remark: Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentraitons (3 nM), ethylhexanol also increased intracellular calcium.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(174)

Type: Biochemical or cellular interactions
Remark: The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(175)

Type: Biochemical or cellular interactions
Remark: Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O2/CO2-saturated buffer. Following infusion of ethylhexanol, O2 uptake and ketone body formation were diminished by 50 and 80%, respectilely, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O2-rich upstream regions of the liver lobule were damaged as reflected by trypan blue uptake. It is concluded, that the

toxicity of ethylhexanol in the liver is dependent on local O2 tension and mitochondria are primary targets.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(176)

Type: Biochemical or cellular interactions

Remark: 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration pereceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl2 by isolated mitochondria 4- to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(177)

Type: Biochemical or cellular interactions

Remark: 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with 2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O2. The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(178)

Type: Biochemical or cellular interactions

Remark: The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanolturned out to be weak.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(179)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activitiy was detected.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(180)

Type: Biochemical or cellular interactions
Remark: Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(181)

Type: Biochemical or cellular interactions
Remark: Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-(2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(100)

Type: Biochemical or cellular interactions
Remark: Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(182)

Type: Biochemical or cellular interactions
Remark: The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a substancial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes, administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(183)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(184)

Type: Biochemical or cellular interactions
Remark: Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(114)

Type: Biochemical or cellular interactions
Remark: The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These

chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(185)

Type: Biochemical or cellular interactions

Remark: In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferaiton in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the immunochemical detectabel levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined. 2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(186)

Type: Biochemical or cellular interactions

Remark: Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse heaptocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxsomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(187)

Type: Biochemical or cellular interactions

Remark: B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were pretrerated for 4 weeks with 1% di(2-ethylhexyl)-phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(167)

Type: Biochemical or cellular interactions
Remark: The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawely rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(168)

Type: Biochemical or cellular interactions
Remark: The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(169)

Type: Biochemical or cellular interactions
Remark: Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the reminder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl -CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(170)

Type: Biochemical or cellular interactions
Remark: Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(171)

Type: Biochemical or cellular interactions
Remark: Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acteyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared to the control.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(172)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(173)

Type: Biochemical or cellular interactions
Remark: Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentraitons (3 nM), ethylhexanol also increased intracellular calcium.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(174)

Type: Biochemical or cellular interactions
Remark: The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(175)

Type: Biochemical or cellular interactions
Remark: Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O2/CO2-saturated buffer. Following infusion of ethylhexanol, O2 uptake and ketone body formation were diminished by 50 and 80%, respectilely, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O2-rich upstream regions of the liver lobule were damaged as reflected by trypan blue uptake. It is concluded, that the toxicity of ethylhexanol in the liver is dependent on local O2 tension and mitochondria are primary targets.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(176)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration pereceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl2 by isolated mitochondria 4- to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(177)

Type: Biochemical or cellular interactions
Remark: 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with

2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O2. The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(178)

Type: Biochemical or cellular interactions

Remark: The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanolturned out to be weak.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(179)

Type: Biochemical or cellular interactions

Remark: 2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activitiy was detected.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(180)

Type: Biochemical or cellular interactions

Remark: Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(181)

Type: Biochemical or cellular interactions

Remark: Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-(2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in

animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(100)

Type: Biochemical or cellular interactions

Remark: Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(182)

Type: Biochemical or cellular interactions

Remark: The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a substancial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes, administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(183)

Type: Biochemical or cellular interactions

Remark: 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.

Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Celanese GmbH Frankfurt am Main

(184)

Type: Biochemical or cellular interactions
Remark: Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(114)

Type: Biochemical or cellular interactions
Remark: The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(185)

Type: Biochemical or cellular interactions
Remark: In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferaiton in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the immunochemical detectabel levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined. 2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(186)

Type: Biochemical or cellular interactions
Remark: Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse heaptocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxsomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(187)

Type: Metabolism
Remark: 2-Ethylhexanol was efficiently absorbed following oral administration to rats. 14C associated with 2-ethyl[1-14C]-hexanol was rapidly excreted in respiratory CO2 ((6-7%), faeces (8-9%) and urine (80-82%), with essentially complete elimination by 28 h after administration.
The amount of label recovered in CO2 matched the amount of unlabelled 2-heptanone plus 4-heptanone recovered from urine, suggesting that both types of metabolites may have been derived from the major urinary metabolite, 2-ethylhexanoix acid, by decarboxylation following partial beta-oxidation. The 14CO2 appeared not to be derived from acetate or by reductive decarboxylation.
Other identified metabolites were 2-ethyl5-hydroxyhexanoic acid, 2-ethyl-5-ketohexanoic acid, and 2-ethyl-1,6-hexene-dioic acid. Only about 3% of the ethylhexanol was excreted unchanged.
Ethylhexanol was a competitive inhibitor of yeast alcohol dehydrogenase, but a good substrate for horse alcohol dehydrogenase.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(188)

Type: Metabolism
Remark: From experiments with perfused livers from starved rats it is concluded that 2-ethylhexanol is oxidized via phenobarbital-inducible pathways to metabolites which do not inhibit ketogenesis and that ethylhexanol inhibits beta-oxidation of fatty acids in mitochondria but not in peroxisomes. Treatment of rats with ethylhexanol (0.32 g/kg i.p.) decreased plasma ketone bodies from 1.6 to 0.8 mM, increased hepatic triglycerides and increased lipid

predominantly in periportal regions of the liver lobule.

Source: Neste Oxo AB Stenungsund

(189)

Type: Metabolism

Remark: Three rabbits were each given 3 ml of 2-ethylhexanol by gavage. Nearly 90% of ethylhexanol was excreted as alpha-ethylhexanoylglucuronide.

Source: Neste Oxo AB Stenungsund

(190)

Type: Metabolism

Remark: From experiments with perfused livers from starved rats it is concluded that 2-ethylhexanol is oxidized via phenobarbital-inducible pathways to metabolites which do not inhibit ketogenesis and that ethylhexanol inhibits beta-oxidation of fatty acids in mitochondria but not in peroxisomes. Treatment of rats with ethylhexanol (0.32 g/kg i.p.) decreased plasma ketone bodies from 1.6 to 0.8 mM, increased hepatic triglycerides and increased lipid predominantly in periportal regions of the liver lobule.

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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(189)

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(190)

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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(189)

Type: Metabolism
Remark: Three rabbits were each given 3 ml of 2-ethylhexanol by gavage. Nearly 90% of ethylhexanol was excreted as alpha-ethylhexanoylglucuronide.
Source: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(190)

Type: Toxicokinetics
Remark: Excretion balance studies were conducted in female Fischer 344 rats with high (500 mg/kg) and low (50 mg/kg) oral doses of [14C]2-ethylhexanol, and following repeated oral dosing at the low level. Dermal exposures were conducted for 6 hrs with a 1 g/kg applied dose of [14C]2-ethylhexanol. The bioavailability of unlabeled 2-ethylhexanol at 500 mg/kg was compared following oral dosing as a neat chemical, and an emulsion in aqueous Cremophore EL. The high, low and repeated low oral doses of 2-ethylhexanol showed similar excretion balance profiles of [14C], with some evidence of metabolic saturation at the high dose. No evidence of metabolic induction was seen following the repeated low oral dosing. All of the oral doses were eliminated rapidly, predominantly in the urine during the first 24 hr following dosing. The dosing resulted in only about 5% absorption of the 1 g/kg dose, with the majority of the dose recovered unabsorbed from the dermal exposure cell at 6 hr. The majority of the oral and dermal doses were eliminated as glucuronides of oxidized metabolites of 2-ethylhexanol. The major urinary metabolites detected were glucoronides of 2-ethyladipic acid, 2-ethylhexanoic acid, and 5-hydroxy-2-ethylhexanoic acid, and 6-hydroxy-2-ethylhexanoic acid. Only trace amounts of unchanged 2-ethylhexanol were seen in urine. The bioavailability of 2-ethylhexanol, as determined by pharmacokinetic analylsis of blood 2-ethylhexanoic acid levels, dosed orally as an emulsion in Cremophor EL, was found to be slightly, but not significantly, greater than 2-ethylhexanol dosed orally as a neat chemical.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(191)

Type: other
Remark: The hypotensive effect of 2-ethylhexanol was tested in rabbits and dogs. 0.002 to 0.032 mmoles/kg 2-ethylhexanol, injected i.v. into Vena jugularis or Vena femoralis, dose dependently decreased the blood pressure of rabbits.The heart rate increased considerably in direct relation to the dosage, as did the frequency of respiration. With dogs, no

consistent hypotensive effects were observed.

Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(192)

5.11 Experience with Human Exposure

Remark: No study located.
Source: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Remark: Es liegen keine Untersuchungsberichte der BASF vor.
Source: BASF AG Ludwigshafen

(1) TRGS 900 (1993)

(2) Huels AG: Sicherheitsdatenblatt "2-Ethylhexanol", Version 11, 17 Feb. 1997

(3) Inhouse data from Neste Oxo AB, Stenungsund.

(4) Bundesminister des Innern (1996): Gemeinsames Ministerialblatt Nr. 16, 47. Jahrgang, 338, Kenn-Nr. 134 (29.04.1996)

(5) Stoerfall-Verordnung vom 20.09.1991

(6) Stoerfallverordnung (1991): Bundesgesetzblatt, Teil 1, Anhang II (28.09.1991)

(7) BASF AG, Sicherheitsdatenblatt 2-Ethylhexanol, 25.01.1996

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Results:	Municipal	Industrial
BOD5/COD	0.70	0.60
BOD10/COD	0.81	0.77
BOD20/COD	0.87	0.86

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7.1 Risk Assessment

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