

I U C L I D

Data Set

Existing Chemical : ID: 149-30-4
CAS No. : 149-30-4
EINECS Name : benzothiazole-2-thiol
EC No. : 205-736-8
TSCA Name : 2(3H)-Benzothiazolethione
Molecular Formula : C7H5NS2

Producer related part
Company : Bayer Corporation
Creation date : 15.07.1999

Substance related part
Company : Bayer Corporation
Creation date : 15.07.1999

Status :
Memo : American Chemistry Council, Rubber and Plastic Additives Panel,
Benzothiazole-based Thiazoles Category

Printing date : 18.06.2003
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Number of pages : 61

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
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Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2. Physico-Chemical Data

Id 149-30-4

Date 18.06.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation
Name : American Chemistry Council - Rubber and Plastics Additives Panel (RAPA)
Contact person :
Date :
Street : 1300 Wilson Boulevard
Town : 22209 Arlington, VA
Country : United States
Phone : 703-741-5600
Telefax : 703-741-6091

26.04.2001

Type : cooperating company
Name : Bayer Polymers LLC (a wholly-owned subsidiary of Bayer Corporation)
Contact person :
Date :
Street : 100 Bayer Road
Town : PA 15205-9741 Pittsburgh
Country : United States

15.05.2003

Type : cooperating company
Name : Crompton Corporation
Contact person :
Date :
Street : Benson Road
Town : 06749 Middlebury, CT
Country : United States

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Type : cooperating company
Name : Flexsys America L.P.
Contact person :
Date :
Street : 260 Springside Drive
Town : 44333-0444 Akron, OH
Country : United States

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Type : cooperating company
Name : Noveon, Inc.
Contact person :
Date :
Street : 9911 Brecksville Road
Town : 44141-3247 Cleveland, OH
Country : United States

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1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

2. Physico-Chemical Data

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1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name : 2(3H)-Benzothiazolethione
Smiles Code : N(c(c(S1)ccc2)c2)=C1S
Molecular formula : C7 H5 N1 S2
Molecular weight : 167.24
Petrol class :

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1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : solid
Purity : > 96 - % w/w
Colour :
Odour :

15.05.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2(3H)-benzothiazolethione

20.10.1999

2-mercaptobenzothiazole

20.10.1999

MBT

20.10.1999

1.3 IMPURITIES

Purity :
CAS-No : 7704-34-9
EC-No : 231-722-6
EINECS-Name : sulphur
Molecular formula :
Value : < 1 - % w/w

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Purity :
CAS-No :
EC-No :
EINECS-Name : N-Phenyl-2-benzothiazolamine
Molecular formula :
Value : < 1 - % w/w

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Purity :
CAS-No : 934-34-9
EC-No : 213-281-1
EINECS-Name : benzothiazol-2(3H)-one
Molecular formula :
Value : < .5 - % w/w

15.05.2003

1.4 ADDITIVES

Purity type :
CAS-No : 8042-47-5
EC-No : 232-455-8
EINECS-Name : White mineral oil (petroleum)
Molecular formula :
Value : 0 - 2 % w/w
Function of additive : Dust control agent

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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

Type : TSCA
Additional information :

15.05.2003

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

2. Physico-Chemical Data

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2.1 MELTING POINT

Value : 181 - °C
Sublimation :
Method : other: Handbook value
Year :
GLP :
Test substance :

Reliability : (2) valid with restrictions
Data from Handbook or collection of data
Flag : Critical study for SIDS endpoint
06.11.2000 (1)

Value : = 180.2 - 181.7 °C
Decomposition : no, at - °C
Sublimation :
Method : other: Handbook value
Year :
GLP :
Test substance :

Source : Bayer AG Leverkusen
Reliability : (2) valid with restrictions
Data from Handbook or collection of data
Flag : Critical study for SIDS endpoint
26.04.2001 (2)

2.2 BOILING POINT

Value : > 260 - °C at 1013 hPa
Decomposition : yes
Method :
Year :
GLP : no data
Test substance : other TS: 2-mercaptobenzothiazole (CAS# 149-30-4); purity not noted

Remark : Decomposes above 260 degrees centigrade.
Source : Bayer AG Leverkusen
Reliability : (3) invalid
Documentation insufficient for assessment
Flag : Critical study for SIDS endpoint
15.05.2003 (3)

2.3 DENSITY

Type : density
Value : = 1.42 - g/cm³ at 20 °C
Method : other: Handbook value
GLP : no data
Test substance :

Source : Bayer AG Leverkusen
Reliability : (2) valid with restrictions
Data from Handbook or collection of data
Flag : Critical study for SIDS endpoint
06.11.2000 (1) (4)

2. Physico-Chemical Data

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2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : < .000003 - hPa at 25 °C
Decomposition :
Method : OECD Guide-line 104 "Vapour Pressure Curve"
Year : 1981
GLP : yes
Test substance :

Remark : Method similar to OECD test method 104. This procedure employed the gas saturation technique.

Source : Bayer AG Leverkusen
Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint

06.11.2000

(5)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : = 2.34 - 2.5 at °C
pH value : -
Method : other (measured)
Year : 1980
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen
Reliability : (2) valid with restrictions
Method did not follow OECD guidelines. Samples analyzed at one test concentration only.

Flag : Critical study for SIDS endpoint

15.05.2003

(6)

Partition coefficient :
Log pow : 2.41 - at °C
pH value : -
Method : other (measured)
Year :
GLP : no data
Test substance : other TS: 2-mercaptobenzothiazole (CAS# 149-30-4); purity not noted

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

15.05.2003

(7)

Partition coefficient :
Log pow : 2.862 - at 25 °C
pH value : -
Method : other (calculated): KOWWIN Program (v1.65)
GLP : no
Test substance : other TS: molecular structure

Reliability : (2) valid with restrictions
Accepted calculation method

15.05.2003

(8)

2. Physico-Chemical Data

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2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in Value : Water
: = 118 - mg/l at 25 °C
pH value : = 7 -
concentration : at °C
Temperature effects : Not measured; pH effect measured
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product : not measured
Method : other: Campbell Method; Campbell A.N., J. Chem. Soc. London, Part I, 179 - 180, 1930
Year : 1980
GLP : yes
Test substance : other TS: As prescribed by 1.1-1.4, purity >97%

Remark : Equilibration was done with the apparatus wrapped in foil to exclude all light and prevent photodegradation.

Result : Water solubility measured at:
pH 5 = 51 ppm
pH 7 = 118 ppm
pH 9 = 900 ppm

Reliability : (2) valid with restrictions
GLP study

Flag : Critical study for SIDS endpoint
16.05.2003 (9)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : ca. 252 °C
Type : open cup
Method : other
Year :
GLP : no data
Test substance :

Source : Bayer AG Leverkusen
19.05.1994 (3)

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. Environmental Fate and Pathways

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3.1.1 PHOTODEGRADATION

Type	:	water	
Light source	:	Sun light	
Light spectrum	:	- nm	
Relative intensity	:	- based on intensity of sunlight	
Conc. of substance	:	.495 mg/l at 36 °C	
DIRECT PHOTOLYSIS			
Halflife t1/2	:	31.1 - minute(s)	
Degradation	:	86 - % after 90 minute(s)	
Quantum yield	:		
INDIRECT PHOTOLYSIS			
Sensitizer	:	water with additives	
Conc. of sensitizer	:		
Rate constant	:	cm ³ /(molecule*sec)	
Degradation	:	= 91 - % after 90 minute(s)	
Deg. product	:		
Method	:	EPA OTS 795.7000	
Year	:	1989	
GLP	:	yes	
Test substance	:	other TS: 2-mercaptobenzothizole; purity = 98.2%	
Method	:	Federal register 53(173) page 34522-34530.	
Test condition	:	Indirect photolysis measurement was with added humic acid. Half-life estimated to be 27.4 minutes.	
Reliability	:	(1) valid without restriction GLP Guideline study	
Flag	:	Critical study for SIDS endpoint	(10)
18.06.2003			
Type	:	air	
Light source	:		
Light spectrum	:	- nm	
Relative intensity	:	- based on intensity of sunlight	
INDIRECT PHOTOLYSIS			
Sensitizer	:	OH	
Conc. of sensitizer	:	1560000 molecule/cm ³	
Rate constant	:	.000000000406348 cm ³ /(molecule*sec)	
Degradation	:	50 - % after 3.2 hour(s)	
Deg. product	:		
Method	:	other (calculated): AOP Program (v1.89)	
Year	:	1999	
GLP	:	no	
Test substance	:	other TS: molecular structure	
Reliability	:	(2) valid with restrictions Accepted calculation method	
Flag	:	Critical study for SIDS endpoint	(8)
15.05.2003			
Type	:	other: dilute phosphate buffer	
Light source	:	Sun light	
Light spectrum	:	- nm	
Relative intensity	:	- based on intensity of sunlight	
Conc. of substance	:	11.1 mg/l at 20 °C	
DIRECT PHOTOLYSIS			
Halflife t1/2	:	.1 - .2 day(s)	
Degradation	:	100 - % after	
Quantum yield	:	0	

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INDIRECT PHOTOLYSIS

Sensitizer : other: dissolved organic matter
Conc. of sensitizer : 10 mg/l
Rate constant : ca. 3.1 cm³/(molecule*sec)
Degradation : 98 - % after
Deg. product : yes
Method : other (measured): test conditions undocumented
Year : 1992
GLP : no data
Test substance : no data

Remark : for direct photolysis:
pH 7, rate constant 8.1-8.7;
for indirect photolysis:
initial conc.=1.9 mg/l, temp=1-10C, total solar radiation=36.3E/m², pH=7, t
1/2=.28-.44 day, quantum yield=.0013;
similar results obtained when natural water was used: quantum yield=.0015
and 100% reduction;
Products formed with and without sensitizer and in natural water:
benzothiazole (28-47%), 2-hydroxybenzothiazole (4-5%) and
unidentified product

Source : Bayer AG Leverkusen

18.06.2003

(11)

Type : other: ethanol
Light source : other: Hanovia mercury lamp-UV irradiation
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
Conc. of substance : 860 mg/l at °C
Method : other (measured): Parkanyi, C. et al protocol; see test conditions
Year : 1985
GLP : no data
Test substance : no data

Remark : Final product was benzothiazole sulfate with solutions of
methanol, ethanol or acetonitrile; When dry benzene or
toluene was the reaction medium bis-(2-benzothiazolyl)
disulfide was formed that could then be degraded to
benzothiazole; oxygen is necessary for this reaction to
take place and water is needed for last step

Source : Bayer AG Leverkusen

Test condition : immersion-well type; water cooled Ace Glass photochemical
reactor; air saturated 96% ethanol; irradiated 22 hours; 450
watts

03.03.1994

(12)

Type : other: filter paper
Light source : other: germicidal lamp
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
Method : other (measured): Mitchell, E.C. protocol; see test conditions
Year : 1961
GLP : no data
Test substance : no data

Remark : classified as "little or no degradation"

Source : Bayer AG Leverkusen

Test condition : 10 mg quantities of a pesticide chemical are spotted on
filter paper and the spot is exposed to a germicidal light
(30 watt)

03.03.1994

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Type : water
Light source : Sun light
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
Conc. of substance : 1.1 mg/l at °C
DIRECT PHOTOLYSIS
Halflife t1/2 : 3.7 - hour(s)
Degradation : - % after
Quantum yield :
Deg. product :
Method : other (measured): test conditions undocumented
Year : 1980
GLP : yes
Test substance : other TS: mecaptobanzothiazole; purity 98%

Remark : Dark control T1/2 = 100 hours.
Four photodegradation by-products were observed.

15.05.2003

(9)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : - at °C
t1/2 pH7 : - at °C
t1/2 pH9 : - at °C
Degradation : 15 - % after 7 day(s) at pH 7 and °C
Deg. product :
Method : other: Monsanto protocol
Year : 1985
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen
Reliability : (1) valid without restriction
GLP study
Flag : Critical study for SIDS endpoint

15.05.2003

(14)

Type : abiotic
t1/2 pH4 : - at °C
t1/2 pH7 : - at °C
t1/2 pH9 : - at °C
Degradation : - 0 % after 7 day(s) at pH and °C
Deg. product :
Method : other: according to Analytic Bio-Chemistry Labs Protocol
Year : 1984
GLP : no data
Test substance : other TS: 2-mercaptobenzothiazole, purity = 98%

Remark : No measurable hydrolysis after 7 days
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment

15.05.2003

(15)

Type : biotic
t1/2 pH4 : - at °C
t1/2 pH7 : - at °C
t1/2 pH9 : - at °C
Deg. product :

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Method : other: test conditions undocumented
Year : 1992
GLP : no data
Test substance : no data

Remark : 6 mg chemical; sediment 1.33 g dry weight/l H₂O; Converted in low yield to 2-(methylthio)benzothiazole

Source : Bayer AG Leverkusen
Reliability : (3) invalid
Documentation insufficient for assessment

15.05.2003

(11)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

Type of measurement : other: monitoring paper mill
Media : other: effluent
Concentration : -
Method :

Remark : 4 samples taken at various stages of treatment; conc. ranged from .025-.035 mg/l

Source : Bayer AG Leverkusen

03.03.1994

(16)

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : adsorption
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 : other: Springborn Laboratories protocol; see test conditions
Year : 1989

Result : Results:

	Kd	Koc	Slope (1/n)	%Organic Matter
California Sandy Loam	4.38	677	0.855	1.1
California Clay Loam	5.73	326	0.808	3.0
California Sand	0.799	1360	1.137	0.1
Carver Sandy Loam	18.8	2130	0.594	1.5
Dartmouth Sand	23.0	3560	0.861	1.1
Weweantic Sand	18.3	2590	0.763	1.2

Kd = adsorption coefficient

Koc = adsorption coefficient based on organic carbon content

Test condition : Protocol followed US TSCA Test Standard 40 CFR Chapter 1, paragraph 796.2750.

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint

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Type : fugacity model level III
Media : other: air, water, soil, sediment
Method : other: EPIWIN Level III Fugacity Model
Year : 1999

Remark : Modeling was performed using equal releases (1,000 kg/hr) and equal distribution to all compartments.

Result :

	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.507	6.32	1000	7.72e-012
Water	35.9	360	1000	4.06e-013
Soil	63.4	360	1000	2.76e-012
Sediment	0.172	1.44e+003	0	2.71e-013

Persistence Time: 347 hr
Reaction Time: 405 hr
Advection Time: 2.44e+003 hr
Percent Reacted: 85.8
Percent Advected: 14.2

Reliability : (2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint
18.06.2003

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Type : adsorption
Media : water - soil
Method :
Year :

Method : Aqueous solutions of MBT, initial concentrations ranging from 0.1 to 1.0 ppm, were equilibrated for 24 hours with four soils. K (adsorption coefficient) was calculated using the following equation
$$K = \frac{\text{equilibrium concentration in soil}}{\text{equilibrium concentration in water}}$$

The concentration in the water was measured using analytical method ES-80-M-15. The concentration in the soil was calculated by the difference.

Result :

Soil	K	95% confidence limits
Drummer silty clay loam	18	13-23
Spinks sandy loam	12	8-19
Ray silt loam	10	6-16
Lintonia sandy loam	7.5	5-11

Mean = 12

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

16.05.2003

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3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 23.8 mg/l related to Test substance
Contact time : 28 days

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Degradation Result : < 1 - (\pm) % after 28 day(s)
Deg. product : under test conditions no biodegradation observed
Method : EPA OTS 796.3100
Year : 1989
GLP : yes
Test substance : other TS: 2-mercaptobenzothiazole, purity = 98%

Remark : Gledhill method listed in U.S. TSCA regulations 40 CFR Ch 1 subpart D paragraph 796.3100

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint

15.05.2003

(19)

Type : aerobic
Inoculum : other: sludge samplings from different sewage plants, rivers, bays and a lake

Concentration : 100 mg/l related to Test substance

Contact time :
Degradation Result : 2.5 - (\pm) % after 14 day(s)

Deg. product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year : 1981
GLP : no data
Test substance : no data

Remark : 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

15.05.2003

(20)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 18 mg/l related to Test substance
Contact time :
Degradation Result : 0 - 5 (\pm) % after 35 day(s)
under test conditions no biodegradation observed

Deg. product :
Method : other: CO₂ evolution method listed in U.S. TSCA regulations 40 CFR Ch 1 subpart D paragraph 796.3100.

Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Sample run in triplicate; 0%, 2%, and 5% theoretical carbon dioxide evolution obtained with an average of 2%.

Source : Bayer AG Leverkusen

Reliability : (1) valid without restriction
Guideline study

15.05.2003

(21)

Type : aerobic
Inoculum : other: water and sediment from nearby creek, agricultural land and industrial site with sediment.

Concentration : 1 mg/l related to Test substance

Contact time :
Degradation : 81 - (\pm) % after 56 day(s)

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Result : other: Primary degradation was estimated to be 81% after 8 weeks. Sterile samples also degraded.
Deg. product :
Method : other: SRI protocol; see test conditions
Year : 1985
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen
Test condition : River die-away test.
18.01.1995 (22)

Type : aerobic
Inoculum : activated sludge
Concentration : 3 mg/l related to Test substance
Contact time :
Degradation : - (\pm) % after
Result : other: 3 mg/l inhibited oxidation of ammonia by 75%.
Deg. product :
Method : other: see test conditions
Year : 1966
GLP : no data
Test substance : no data

Remark : The concentration of the oxidized form, benzothiazole disulphide, had to be about 10 times greater than that of MBT to give 75% inhibition of ammonia oxidation.

Source : Bayer AG Leverkusen
Test condition : 250 ml flasks at 25 degrees Celsius shaker for 2-4 hours.
18.01.1995 (23)

Type : aerobic
Inoculum : activated sludge
Concentration : 5 mg/l related to Test substance
Contact time :
Degradation : - (\pm) % after
Result : other: 74% inhibition of the nitrifying activity of activated sludge
Deg. product :
Method : other: see test conditions
Year : 1966
GLP : no data
Test substance : no data

Remark : 5 mg/l MBT produced 74% inhibition, but in the presence of 5 mg/l zinc as zinc sulphate, which itself was not inhibitory, MBT was noninhibitory.

Source : Bayer AG Leverkusen
Test condition : 250 ml flasks at 25C in a shaker for 2-4 hours.
26.04.1994 (23)

Type : aerobic
Inoculum : activated sludge
Concentration : 20 mg/l related to Test substance
Deg. product :
Method : other: see test conditions
Year : 1966
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen
Test condition : Sewage containing MBT was supplied daily to a fill-and-draw plant. Initial period of 9 weeks MBT conc 2 mg/L, was

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increased to 20 mg/L for 7 weeks. Results suggest that during experiment, a strain of Nitrosomonas developed which was far less susceptible to MBT than that in the control sludge. Whereas 2 mg/L MBT inhibited control sludge by 75%, over 40 mg/L was necessary to produce the same effect on sludge which was previously exposed to 20 mg/L MBT. There was no evidence MBT was being decomposed in the sewage.

03.03.1994

(23)

Type : aerobic
Inoculum : other: soil
Concentration : 1 g/l related to Test substance
Contact time :
Degradation : - (\pm) % after
Result : other: completely retarded microbial growth of soil microbes at 0.1%
Deg. product :
Method : other: see test conditions
Year : 1984
GLP : no data
Test substance : no data

Remark : After three months, MBT completely retarded microbial growth of soil microbes at 0.1%. Toxicity level for MBT in agar: 4-day LD50 & 14-day LD50 \leq 0.1%.

Source : Bayer AG Leverkusen
Test condition : Three techniques used for exposing rubber additives to John Innes No. 1 Soil. 1st involved placing powdered additives onto non-biodegradable polycarbonate membranes w/a 12 μ m pore diameter & placing membranes onto the soil w/powders on the upper surface. 2nd involved embedding powdered additives onto a thin layer (0.3 cm) of epoxy resin poured onto aluminum foil. During the curing process, excess of powder was poured onto resin. When cured, excess powder was shaken off resin which was cut and placed with the additive in contact with the soil. 3rd technique involved incorporating additives into an agar medium & inoculating medium with soil extract.

26.04.1994

(24)

Type : aerobic
Inoculum :
Concentration : 20 mg/l related to Test substance
Contact time :
Degradation : 0 - 12 (\pm) % after 3 day(s)
Result :
Deg. product :
Method : other: see test conditions
Year :
GLP : no data
Test substance : no data

Remark : 2-MBT was tested for degradability in river water by 4 different institutes. The results were 0%, 3%, 11% & 12%. It was also tested in sea water with the following results: 0%, 21%, 41%, 10%.

Partial translation (abstract and results table) of a Japanese article.

Source : Bayer AG Leverkusen
Test condition : Method was listed as the "cultivation method".

18.01.1995

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Type : aerobic
Inoculum :
Contact time :
Degradation : - (\pm) % after
Result : other: listed as resistant substance in U.K.
Deg. product :
Method : other: test conditions undocumented
Year : 1975
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen (26)
03.03.1994

Contact time :
Degradation : - (\pm) % after
Result : other: listed as degradation resistant
Deg. product :
Method : other: MITI
Year :
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen (27)
26.04.1994

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species : Cyprinus carpio (Fish, fresh water)
Exposure period : 42 day(s) at °C
Concentration : .1 mg/l
BCF : < .8 -
Elimination : no data
Method : OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year : 1981
GLP : no data
Test substance : no data

Remark : when test conc. .01 mg/l BCF < 8.0
Source : Bayer AG Leverkusen
Reliability : (1) valid without restriction
Guideline study
15.05.2003 (20)

Species : Cyprinus carpio (Fish, fresh water)
Exposure period : at 15 °C
Concentration : .56 mg/l
Elimination : yes
Method : other: Hashimoto, K. et al protocol; see test conditions
Year : 1978
GLP : no data
Test substance : other TS: 14C; 98.5% pure

Remark : about 20% excreted at 1h, 35% at 2h, 75% at 24h and 77% at 72h; fish that were fed had 100% excretion at 72hr; chemical oxidized to C-2,2,dithiobis[benzothiazole]
Source : Bayer AG Leverkusen
Test condition : fish starved 2 days prior to test; 30L water; water renewed at periodic intervals, some fish fed after administration of

3. Environmental Fate and Pathways

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15.05.2003 chemical, chemical administered with a catheter into intestine (28)

Species : Cyprinus carpio (Fish, fresh water)
Exposure period : 56 day(s) at 25 °C
Concentration :
Elimination : no data
Method : other: test conditions undocumented
Year : 1978
GLP : no data
Test substance : no data

Remark : "confirmed to be non accumulative or low accumulative" ie. BCF did not increase a few hundred times during the 56 day exposure

Source : Bayer AG Leverkusen
Test condition : length 10 cm; weight 30 g; DO 7 mg/l
Reliability : (3) invalid
Documentation insufficient for assessment

15.05.2003 (29)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 149-30-4

Date 18.06.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : 4.2 -
LC50 : 11 -
Limit test :
Analytical monitoring : no
Method : OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year : 1984
GLP : yes
Test substance : other TS: 2-mercaptobenzothiazole, purity = 98%

Remark : all conc. tested were above solubility
C.I. 8.3-15 mg/l; 24h-LC50: 18 mg/l; 48h-LC50: 13mg/l

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint

15.05.2003

(30)

Type : static
Species : Brachydanio rerio (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC0 : .8 -
LC100 : 3.2 -
Limit test :
Analytical monitoring : yes
Method : other: UBA-Verfahrensvorschlag "Lethale Wirkung beim
Zebrabaerbling Brachydanio rerio (LC0, LC50 < LC100, 48-96 h), Mai 1984
Year : 1984
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : geometric mean: 1.6 mg/l

Source : Bayer AG Leverkusen

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint

15.05.2003

(31)

Type : flow through
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 8 day(s)
Unit : mg/l
NOEC : 2 -
LC50 : .67 -
Limit test :
Analytical monitoring : yes
Method : other: Springborn Laboratory protocol; see test conditions
Year : 1981
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : C.I. 0.54-0.83 mg/l; 24h-LC50: 1.14 mg/l; 48h-LC50: 0.73
mg/l

Source : Bayer AG Leverkusen

4. Ecotoxicity

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Test condition : continuous flow; 19L aquaria; 10 fish/conc; fed brine shrimp daily
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
15.05.2003 (32)

Type : static
Species : Lepomis macrochirus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : 1.5 -
Limit test :
Analytical monitoring : no
Method : other: Bionomics Laboratroy protocol; see test conditions
Year : 1976
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : C.I. 1.2-1.9 mg/l; 24h-LC50: 3.4 mg/l; 48h-LC50: 2.1 mg/l
Source : Bayer AG Leverkusen
Test condition : carrier-acetone; 15L water; 10 fish/vessel; length 3.8 cm; no food; no aeration; temp 22 degrees Celsius
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
15.05.2003 (33)

Type : static
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : .75 -
Analytical monitoring : no
Method : other: Bionomics Laboratory protocol; see test conditions
Year : 1976
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : C.I. 0.55-1 mg/l; 24h-LC50: 0.92 mg/l; 48h-LC50: 0.75 mg/l
Test condition : carrier-acetone; 15L water; 10 fish/vessel; length 3.7 cm; no food; no aeration; temp 12 degrees Celsius
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
15.05.2003 (34)

Type : semistatic
Species : Cyprinus auratus
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : 2 -
Analytical monitoring : no data
Method : other: test conditions undocumented
Year : 1983
GLP : no data
Test substance : no data
Source : Bayer AG Leverkusen
Reliability : (3) invalid
Documentation insufficient for assessment
15.05.2003 (35)

4. Ecotoxicity

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Date 18.06.2003

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : 1.9 -
EC50 : 2.9 -
Analytical monitoring : yes
Method : other: "Protocol for Conducting a Static Acute Toxicity Test with Daphnia magna Following FIFRA Guideline 72", SLI Protocol #010190/FIFRA 72-2 DM SA and protocol amendment #1 dated 9 January 1992
Year : 1992
GLP : yes
Test substance : other TS: 100 % (2-Mercaptobenzothiazole (ROKON), Lot #N9H 211)
Remark : 24h-EC 50: 3.9 mg/l
Analytical monitoring: HPLC
Reliability : (1) valid without restriction
GLP Guideline study
Flag : Critical study for SIDS endpoint
16.05.2003 (36)

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : 1.8 -
EC50 : 4.1 -
Analytical monitoring : no
Method : other: Methods of Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians, 1975, EPA 660/3-75009
Year : 1975
GLP : yes
Test substance : other TS: As prescribed by 1.1-1.4, purity = 98%
Remark : An initial rangefinding experiment preceded the definitive test.
Concentrations of the test substance (0, 1.0, 1.8, 3.2, 5.6 and 10.0 mg/l) were prepared in reagent-grade acetone. Acetone was used as the solvent control. Water quality parameters of temperature, dissolved oxygen, pH, hardness and alkalinity were monitored throughout the test and remained within acceptable limits. The EC50 value and 95% confidence limits were calculated using the statistical methods of Litchfield and Wilcoxon (1949).
Result : EC50 (24h) = 7.0 mg/l
EC50 (48h) = 4.1 mg/l (C.I. for EC50: 3.6-4.7 mg/l)
NOEC = 1.8 mg/l
Reliability : (1) valid without restriction
GLP Guideline study
Flag : Critical study for SIDS endpoint
18.06.2003 (37)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : biomass
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : .25 -
Analytical monitoring : no

4. Ecotoxicity

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Date 18.06.2003

Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year : 1984
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Biomass 96 hr EC50 = 0.25 mg/l C.I. 0.06-0.98 mg/l;

in vivo chlorophyll results:
24 hr EC50 = >0.3<0.6 mg/l
48 hr EC50 = >0.3<0.6 mg/l
96 hr EC50 = 0.23 mg/l

Test condition : temp 24 degrees Celsius; 4000 lux; Algal Assay Media; init.
inoc. 10000 cells/ml; "cool" white lights

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint
18.06.2003

(38)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic
Species : Tetrahymena sp. (Protozoa)
Exposure period : 24 hour(s)
Unit : mg/l
EC50 : 10 -
Analytical monitoring : no
Method : other: Yoshioka, Y. protocol; see test conditions
Year : 1985
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen
Test condition : temp. 30 degrees Celsius; sterile medium of 2% protose
peptone; 60 umol/l; no agitation; count cell numbers; conc.
ratio of 1.8 in 10 ml media

18.01.1995

(39)

Type : other: undefined and synthetic media
Species : other bacteria: several genera
Exposure period :
Unit :
Analytical monitoring : no data
Method : other: test conditions undocumented
Year : 1976
GLP : no data
Test substance : no data

Remark : complete inhibition at 50-1000 ug/ml; partial inhibition
from 25-1000 ug/ml
Source : Bayer AG Leverkusen
18.01.1995

(40)

Type : other: unknown
Species : Aspergillus niger (Fungi)
Exposure period :
Unit :
Analytical monitoring : no data
Method : other: test conditions undocumented
Year : 1975
GLP : no data

4. Ecotoxicity

Id 149-30-4

Date 18.06.2003

Test substance : no data
Remark : Inhibits sporulation; also inhibits several other bacteria
Source : Bayer AG Leverkusen
04.05.1994 (41)

4.5.1 CHRONIC TOXICITY TO FISH

Species : Oncorhynchus sp.
Endpoint : other: embryo survival,viability, length
Exposure period : 89 day(s)
Unit : mg/l
MATC : .041 - .078
Analytical monitoring : yes
Method : other: according to Federal Register 50:797.1600
Year : 1989
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : max. accept. tox. concentration for larval length; no effect on embryo viability or survival.
Test condition : test lasted 60 days post hatch; 24-80 foot candles; temp. 12 degrees Celsius
Reliability : (1) valid without restriction
GLP Guideline study
15.05.2003 (42)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)
Endpoint : reproduction rate
Exposure period : 21 day(s)
Unit : mg/l
NOEC : .34 -
EC50 : > .47 -
Analytical monitoring : yes
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year : 1989
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Maximum accept. conc.>0.25<0.47 mg/l; geometric mean: 0.34 mg active ingredient/liter
Test condition : carrier acetone; 50% dilutions; 1.8L vessels; 30-70 foot candles; 16 hours light; temp. 20 degrees Celsius
Reliability : (1) valid without restriction
GLP Guideline study
15.05.2003 (43)

Species : Daphnia magna (Crustacea)
Endpoint : reproduction rate
Exposure period : 21 day(s)
Unit : mg/l
NOEC : ca. .22 -
EC50 : ca. 2.22 -
Analytical monitoring : no
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"

4. Ecotoxicity

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Date 18.06.2003

Year : 1987
GLP : no
Test substance : other TS: 99.45 %

Source : Bayer AG Leverkusen
Test condition : concentrations tested: 0.07, 0.22, 0.7, 2.22, and 7 mg/l.
Preparation of stock solution: 100 mg of test substance were weighed into 1 l of water and dissolved over night by means of a magnetic stirrer.

Reliability : (1) valid without restriction
Guideline study

15.05.2003

(31)

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. Toxicity

Id 149-30-4

Date 18.06.2003

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : = 3800 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 20
Vehicle : other: Corn Oil (20% suspension)
Doses : 3160, 3980, 5010 or 6310 mg/kg bw
Method : other: Single Oral Dose, Younger Laboratories Protocol, 1975
Year : 1975
GLP : no data
Test substance : other TS: As prescribed by 1.1-1.4; purity = 98%

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

Flag : Critical study for SIDS endpoint
16.05.2003 (44)

Type : LD50
Value : = 2830 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 20
Vehicle : other: Corn Oil (20% suspension)
Doses : 2000, 2510, 3160 or 3980 mg/kg bw
Method : other: Single Oral Dose, Younger Laboratories Protocol
Year : 1973
GLP : no data
Test substance : other TS: as prescribed by 1.1 - 1.4; purity >97%

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
16.05.2003 (45)

Type : LDLo
Value : = 7500 - 8750 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 5
Vehicle : other: Water (25% aqueous suspension)
Doses : 5.0, 6.25, 7.5, 8.75 or 10.0 g/kg bw
Method : other: Minimum Lethal Dose Protocol, Scientific Associates
Year : 1955
GLP : no data
Test substance : other TS: as prescribed by 1.1 - 1.4; purity = Commercial grade

16.05.2003 (46)

Type : LD50
Value : > 500 - mg/kg bw
Species : rat

5. Toxicity

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Date 18.06.2003

Strain :
Sex : no data
Number of animals :
Vehicle : no data
Doses :
Method :
Year :
GLP :
Test substance : other TS: 2-mercaptobenzothiazole (purity not noted)

15.05.2003 (47)

Type : LD50
Value : 2000 - mg/kg bw
Species : mouse
Strain :
Sex : male
Number of animals :
Vehicle : other: 0.5% carboxymethyl cellulose in normal saline
Doses :
Method :
Year :
GLP :
Test substance : other TS: ROTAX (purified MBT)

Method : Mice were observed for 72 hours after a single oral exposure. LD50 values were calculated by the Cornfield and Mantel modification (1950) of the Karber method.

15.05.2003 (48)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Value : > 1.27 - mg/l
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Exposure time : 4 hour(s)
Method : other: IBT protocol
Year : 1977
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment; age of study, lack of details

18.06.2003 (49)

Type : LC50
Value : > .722 - mg/l
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :

5. Toxicity

Id 149-30-4

Date 18.06.2003

Exposure time : 7 hour(s)
Method : other: Acute Inhalation Toxicity
Year : 1961
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment; age of study, lack of details

18.06.2003

(50)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > 7940 - mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 3
Vehicle : other: Corn Oil (40% suspension)
Doses : 5010 or 7940 mg/kg bw
Method : other: Single Dermal Dose, Younger Laboratories Protocol
Year : 1975
GLP : no data
Test substance : other TS: As prescribed by 1.1-1.4, purity = 98%

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

Flag : Critical study for SIDS endpoint

16.05.2003

(44)

Type : LD50
Value : > 7940 - mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 3
Vehicle : other: Corn Oil (40% suspension)
Doses : 5010 or 7940 mg/kg bw
Method : other: Single Dermal Dose, Younger Laboratories Protocol
Year : 1973
GLP : no data
Test substance : other TS: as prescribed by 1.1 - 1.4; purity >97%

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

16.05.2003

(51)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : LD50
Value : 437 - mg/kg bw
Species : mouse
Strain :

5. Toxicity

Id 149-30-4

Date 18.06.2003

Sex : male
Number of animals :
Vehicle : other: 0.5% carboxymethyl cellulose in normal saline
Doses :
Route of admin. : i.p.
Exposure time :
Method :
Year :
GLP :
Test substance : other TS: ROTAX (purified MBT)

Method : Mice were observed for 72 hours after a single i.p. injection. LD50 values were calculated by the Cornfield and Mantel modification (1950) of the Karber method.

03.11.2000 (48)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 6
Vehicle : other: Water (0.5g test compound moistened with water)
PDII : 0
Result : not irritating
Classification : not irritating
Method : Draize Test
Year : 1975
GLP : no data
Test substance : other TS: As prescribed by 1.1-1.4; purity = 98%

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

16.05.2003 (44)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : not irritating
Classification :
Method :
Year : 1973
GLP :
Test substance : as prescribed by 1.1 - 1.4

15.05.2003 (52)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : 100 other: mg

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Date 18.06.2003

Exposure time : 24 hour(s)
Comment : not rinsed
Number of animals : 6
Vehicle : none
Result : slightly irritating
Classification : not irritating
Method : Draize Test
Year : 1975
GLP : no data
Test substance : other TS: As prescribed by 1.1-1.4, purity = 98%

Remark : Test substance, as a finely ground powder, was introduced into one eye of each animal; the other eye was left untreated and served as a control. Scoring was done via the Draize Method. Score was 3.2 / 110.0 (Slightly irritating).

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

18.06.2003 (44)

Species : rabbit
Concentration :
Dose :
Exposure time :
Comment :
Number of animals :
Vehicle :
Result : not irritating
Classification :
Method : other
Year : 1973
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen
15.05.2003 (52)

5.3 SENSITIZATION

Type : Buehler Test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : OECD Guide-line 406 "Skin Sensitization"
Year : 1992
GLP : no data
Test substance : other TS: 98 % purity

Source : Bayer AG Leverkusen
Reliability : (1) valid without restriction
Guideline study

18.06.2003 (53)

Type : Buehler Test
Species : guinea pig
Number of animals :
Vehicle : petrolatum
Result : sensitizing

5. Toxicity

Id 149-30-4

Date 18.06.2003

Classification :
Method : other
Year : 1988
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : 0/10 animals reacted to 0.1%, 2/10 reacted to 0.5%, 7/10 reacted to 2%.
15.05.2003 (54)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : OECD Guide-line 406 "Skin Sensitization"
Year : 1992
GLP : no data
Test substance : other TS: 98 % purity

Source : Bayer AG Leverkusen
01.09.1994 (53) (55) (56)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification : sensitizing
Method : other
Year : 1970
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen
23.02.1994 (57)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification : sensitizing
Method : other
Year : 1968
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen
23.02.1994 (58)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method :
Year : 1992
GLP : no data
Test substance : no data

5. Toxicity

Id 149-30-4

Date 18.06.2003

Source : Bayer AG Leverkusen (59)
01.09.1994

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method :
Year : 1972
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen (60)
06.09.1994

Type : Mouse local lymphnode assay
Species : mouse
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : other
Year : 1993
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen (61)
02.09.1994

Type : Mouse local lymphnode assay
Species : mouse
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : other: Skin Sensitization Test
Year : 1992
GLP : no data
Test substance : other TS: 98 % purity; dissolved in dimethyl formamide

Source : Bayer AG Leverkusen (53) (55) (56)
01.09.1994

Type : Mouse local lymphnode assay
Species : mouse
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method :
Year : 1989
GLP : no data
Test substance : other TS: dissolved either in DMSO or aqueous solvent

Source : Bayer AG Leverkusen (62)
01.09.1994

Type : Patch-Test
Species : human
Number of animals :

5. Toxicity

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Date 18.06.2003

Vehicle :
Result : not sensitizing
Classification : not sensitizing
Method : other
Year : 1976
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen
23.02.1994 (63)

Type : other
Species : other
Number of animals :
Vehicle :
Result :
Classification :
Method : other
Year : 1987
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : No T-cell response was noted in an in-vitro lymphocyte transformation assay.

Source : Bayer AG Leverkusen
02.06.1994 (64)

Type : other: occlusive epicutaneous test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : other: Skin Sensitization Test according to Brulos
Year : 1976
GLP : no data
Test substance : no data

Remark : Animals were applied 0.5 g test substance (in 1 % vaseline) to the interscapular region on alternate days for 4 weeks (10 applications, occlusive). At the first day of week 1 and 2, 0.1 ml Freund's adjuvans was injected intradermally. One week after the last application animals were challenged with 0.5 g test compound epicutaneously (occlusive). The mean sensitizing index was 1.1 of 3.0 (maximal score). 50 % of animals were sensitized. Test substance was considered to be moderate sensitizing.

Source : Bayer AG Leverkusen
01.09.1994 (65)

5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : 4 weeks
Frequency of treatm. : ad libitum
Post exposure period :

5. Toxicity

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Date 18.06.2003

Doses : 5000, 10000, 15000, 20000, or 25000 ppm (57, 714, 1071, 1429, 1786 mg/kg bw/d)
Control group : yes
NOAEL : = 714 - mg/kg bw
LOAEL : = 1071 - mg/kg bw
Method : other
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : 5000, 10000, 15000, 20000, 25000 ppm = 57, 714, 1071, 1429, 1786 mg/kg bw/d (conversion factor is 14)

Result : Dose: Observations
5000 ppm: NOEL; no effect
10000 ppm: NOEL; no effects
15000 ppm: LOEL; decr bw gain (male); decr food consumption
20000 ppm: decr bw gain; decr food consumption
25000 ppm: decr bw gain; decr food consumption

Source : Bayer AG Leverkusen
Reliability : (1) valid without restriction
GLP study

Flag : Critical study for SIDS endpoint

15.05.2003

(66)

Type : Sub-chronic
Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 13 weeks
Frequency of treatm. : 5 days/week
Post exposure period : 3 days
Doses : 0, 188, 375, 750, 1500, or 3000 mg/kg bw
Control group : yes
NOAEL : = 375 - mg/kg bw
LOAEL : = 750 - mg/kg bw
Method : other
Year :
GLP : yes
Test substance : other TS: mecaptopbenzothizole, purity = 96.3%

Remark : Because the hepatomegaly was not associated with histopathological findings, those dose levels with hepatomegaly but no other toxicity findings are considered to be no observable adverse effect levels (NOAELs) and are reported as NOELs.

Result : Dose: Observations
188 mg/kg bw/d: hepatomegaly, (female)
375 mg/kg bw/d: NOAEL; hepatomegaly, (female)
750 mg/kg bw/d: LOAEL; bw, decr; hepatomegaly, (female)
1500 mg/kg bw/d: bw, decr; hepatomegaly.

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

15.05.2003

(67) (68)

Type :
Species : rat
Sex : male/female

5. Toxicity

Id 149-30-4

Date 18.06.2003

Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : 4 weeks
Frequency of treatm. : continuous
Post exposure period :
Doses : 4300, 9000, 14000, 19000, 25000 ppm
Control group : yes, concurrent vehicle
Method : other
Year :
GLP : no data
Test substance : other TS: 2-mercaptobenzothiazole (lot No. N8F-228)

Method : 2-mercaptobenzothiazole (lot No. N8F-228) was administered to Sprague-Dawley rats at target levels of 0, 5000, 10000, 15000, 20000, 25000 ppm in feed for 4 weeks. The test material was analysed neat and mixed with the diet. Averages for consumption were 425, 839, 1232, 1696, 2143 mg/kg (males) and 432, 874, 1320, 1703, 2058 mg/kg (females).

All animals were observed twice daily for mortality and moribundity. Detailed clinical observations and body weights were done weekly. All animals were given a thorough necropsy and livers were weighed.

Result : Observations included decreased weight gain and reduced food consumption, which were statistically significant in males at 15000 ppm and females at 20000 and 25000 ppm. Slightly heavier livers occurred in animals of both sexes at all levels.

15.05.2003

(69)

Type : Sub-chronic
Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 13 weeks
Frequency of treatm. : 5 days/week
Post exposure period : 3 days
Doses : 94, 188, 375, 750, or 1500 mg/kg bw
Control group : yes
NOAEL : = 375 - mg/kg bw
LOAEL : = 750 - mg/kg bw
Method : other: well documented in Physiological Research Laboratories 78-60-106002 (1981)
Year :
GLP : yes
Test substance : other TS: mecaptobenzothizole, purity = 96.3%

Result : Dose: Observations
94 mg/kg bw/d: no effects
188 mg/kg bw/d: no effects
375 mg/kg bw/d: NOEL; no effects
750 mg/kg bw/d: LOEL; death (female)
1500 mg/kg bw/d: deaths.

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

18.06.2003

(67) (70)

5. Toxicity

Id 149-30-4

Date 18.06.2003

Type :
Species : mouse
Sex : male/female
Strain : other: Slc: ddY
Route of admin. : oral feed
Exposure period : 20 months
Frequency of treatm. : daily
Post exposure period :
Doses : 30, 120, 480 or 1920 ppm (males: 3.6, 14.7, 57.9 or 289.4 mg/kg bw day; females: 3.6, 13.5, 58.9 or 248.0 mg/kg bw/day)
Control group : yes
NOAEL : = 120 - ppm
Method : other: Repeated Dose Toxicity
Year : 1989
GLP : no data
Test substance : other TS: technical grade

Result : Inhibition of body weight gain was observed in the 1920 ppm-group of males from the initial stage of the treatment. No significant changes were seen between the controls and the treated groups in weights of organs and in several biochemical parameters of serum. Histopathologically, cell infiltration in the interstitium of kidney in the 1920 and 480 ppm groups of the males was found at the 20th month.

Source : Bayer AG Leverkusen
18.06.2003

(71)

Type :
Species : mouse
Sex : male
Strain : other: white
Route of admin. : i.p.
Exposure period : 1 week
Frequency of treatm. : daily
Post exposure period : none
Doses : 55 and 110 mg/kg
Control group : yes, concurrent vehicle
NOAEL : 55 - mg/kg bw
LOAEL : 110 - mg/kg bw
Method : other
Year :
GLP :
Test substance : other TS: ROTAX (purified MBT)

Method : Groups of male mice were dosed daily for one week by the i.p. route with oil suspensions of MBT. Control animals received daily injections of the same volume of cottonseed oil. At the end of one week, the animals were sacrificed, tissues were removed and examined histopathologically.

Result : There were no gross signs of toxicity at either dose level. All animals exhibited normal weight gain and behavior. Gross examination at necropsy revealed no significant injury to the vital organs. Microscopic examination of lungs, heart, thyroid and testes were normal. The kidney showed cloudy swelling and the livers revealed severe damage at the 110 mg/kg dose level.

15.05.2003

(48)

5. Toxicity

Id 149-30-4

Date 18.06.2003

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimuriumTA 97, TA98, TA100, TA102
Test concentration : 1, 10, 100, 500, 1000, 5000 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1983
GLP : yes
Test substance : other TS: MBT (purity not noted)

Result : There was no significant increase in revertant colonies and therefore no evidence for mutagenic activity in these assays. There was a toxic response to the test material at 5000 ug/plate and in most cases at 1000 ug/plate. The positive and negative controls were within acceptable limits.

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint

15.05.2003

(72)

Type : HGPRT assay
System of testing : Chinese Hamster Ovary cells
Test concentration : up to 333.33 ug/ml with S9 and up to 33.33 ug/ml without S9
Cycotoxic concentr. : with metabolic activation = 1000 ug/ml;
without metabolic activation = 333.33 ug/ml
Metabolic activation : with and without
Result : negative
Method : EPA OTS 798.5300
Year : 1986
GLP : yes
Test substance : other TS: MBT; lot #39-14B; purity not noted

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint

15.05.2003

(73)

Type : Mouse lymphoma assay
System of testing : L5178Y mouse lymphoma cells
Test concentration : up to 60ug/ml (with) and 70 ug/ml (without)
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 476
Year : 1984
GLP : no data
Test substance : other TS: 2-mercaptobenzothiazole (purity not stated)

Reliability : (1) valid without restriction
Guideline study

15.05.2003

(74)

Type : Sister chromatid exchange assay
System of testing : Chinese hamster ovary cells
Test concentration : up to 500.5 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without

5. Toxicity

Id 149-30-4

Date 18.06.2003

Result : negative
Method : other: BrdUrd/dye technique
Year : 1988
GLP : no data
Test substance : no data

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

15.05.2003 (67)

Type : Cytogenetic assay
System of testing : Chinese hamster ovary cells
Test concentration : up to 500.5 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result :
Method : other: Chromosome Aberration Test
Year : 1988
GLP : no data
Test substance : no data

Remark : result: negative (-S9 mix)
positive at > = 373,5 ug/ml (+ S9 mix)

Source : Bayer AG Leverkusen
15.05.2003 (67)

Type : Mouse lymphoma assay
System of testing : L5178Y
Test concentration : up to 150 ug/ml with S9 and up to 100 ug/ml without S9
Cycotoxic concentr. :
Metabolic activation : with and without
Result : ambiguous
Method : EPA OTS 798.5300
Year : 1986
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : Small increases in mutant frequency were observed but only at concentrations that also produced cytotoxicity.

Reliability : (1) valid without restriction
GLP Guideline study
15.05.2003 (75)

Type : Ames test
System of testing : TA98, TA100, TA1535, TA1537, TA1538
Test concentration : up to 500 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other
Year : 1976
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen
15.05.2003 (76)

Type : Ames test
System of testing : TA98, TA100, TA1535, TA1537, TA1538
Test concentration : up to 300 ug/plate

5. Toxicity

Id 149-30-4

Date 18.06.2003

Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : EPA OTS 798.5265
Year : 1986
GLP : yes
Test substance : other TS: MBT; lot #39-14B; purity = 98%

Reliability : (1) valid without restriction
GLP Guideline study

16.05.2003

(77)

Type : Escherichia coli reverse mutation assay
System of testing : Escherichia coli SD-4-73
Test concentration : no data
Cycotoxic concentr. :
Metabolic activation : without
Result : negative
Method : other: Paper Disk Method
Year : 1958
GLP : no data
Test substance : no data

15.05.2003

(78)

Type : Gene mutation in Saccharomyces cerevisiae
System of testing : D4 strain
Test concentration : up to 500 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other
Year : 1976
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer AG Leverkusen

15.05.2003

(76)

Type : HGPRT assay
System of testing : V79 Chinese hamster cells
Test concentration : 50 - 300 ug/ml
Cycotoxic concentr. :
Metabolic activation : without
Result : negative
Method : other: 6-thioguanine Resistance Assay
Year : 1976
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen

15.05.2003

(79)

Type : Mouse lymphoma assay
System of testing : L5178Y
Test concentration : up to 100 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other
Year : 1978
GLP : no data

5. Toxicity

Id 149-30-4

Date 18.06.2003

Test substance : as prescribed by 1.1 - 1.4
16.05.2003 (80)

Type : Mouse lymphoma assay
System of testing : L5178Y
Test concentration : 3.75 - 150 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result :
Method : other: TK Test
Year : 1985
GLP : yes
Test substance : other TS: solvent: DMSO

Remark : - S9: 1.8- to 8.7fold increases in the mutant frequency for treatments causing very high toxicity (less than 10 % relative growth).
+ S9: 1.7- to 2.7fold increases in the mutant frequency in the 7 - 20 % relative growth range; treatments with 150 ug/ml were lethal.
The results were evaluated as showing the test material to be weakly mutagenic at high toxicity.

Source : Bayer AG Leverkusen
15.05.2003 (81)

Type : Mouse lymphoma assay
System of testing : L5178Y
Test concentration : up to 150 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result :
Method : other: TK Test
Year : 1985
GLP : no data
Test substance : other TS: dissolved in ethanol

Remark : result: negative (- S9 mix)
positive at > = 5 ug/ml (+ S9 mix)

Source : Bayer AG Leverkusen
15.05.2003 (82)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Dominant lethal assay
Species : rat
Sex : male
Strain : CD-1
Route of admin. : oral feed
Exposure period : 13 weeks
Doses : 2500, 8750, or 15000 ppm
Result : negative
Method : EPA OPPTS 870.5450
Year : 1991
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Result : There were no findings that were indicative of dominant lethality.

Reliability : (1) valid without restriction

5. Toxicity

Id 149-30-4

Date 18.06.2003

Flag : GLP Guideline study
15.05.2003 : Critical study for SIDS endpoint (83)

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : CD-1
Route of admin. : i.p.
Exposure period : single dose
Doses : 300 mg/kg bw
Result : negative
Method : EPA OTS 798.5395
Year : 1986
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Result : There was no increase in micronucleated cells as compared to control. MBT was considered not to be clastogenic in this assay.

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint
19.05.2003 (84)

Type : other: In vivo DNA binding study
Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : single dose
Doses : 375 mg/kg
Result : negative
Method : other
Year :
GLP :
Test substance : other TS: radio-labelled 2-mercaptobenzothiazole (purity not noted)

Method : Male and female Fischer 344 rats were gavaged with 375 mg/kg MBT and sacrificed 8 hours later. DNA was extracted from the liver, adrenal glands, pituitary gland, pancreas, and bone marrow using standard exhaustive solvent extraction techniques. The amount of radioactivity associated with the DNA was determined.

Result : There was little or no binding of MBT with DNA in any of the tissues examined.
15.05.2003 (85)

Type : other: Drosophila mutagenicity assay
Species : Drosophila melanogaster
Sex : no data
Strain : no data
Route of admin. : oral feed
Exposure period : 8 - 10 days
Doses : 20 - 40 mg/ml
Result :
Method : other: no data
Year : 1968
GLP : no data
Test substance : no data

Remark : The mutagenic activity included lethal, sublethal and visible mutations.

5. Toxicity

Id

Date 18.06.2003

Result : mutation frequency: 2.5 +- 0.49 %;
no control group mentioned
Source : Bayer AG Leverkusen
15.05.2003

(86)

5.7 CARCINOGENICITY

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 2 years
Frequency of treatm. : 5 days/week
Post exposure period :
Doses : 0, 375 or 750 mg/kg bw for males; 0, 188 or 375 mg/kg bw for females
Result :
Control group : yes
Method : other
Year : 1988
GLP : yes
Test substance : other TS: as prescribed by 1.1 - 1.4; purity = 98%

Remark : The NTP report concluded that "there was some evidence of carcinogenic activity" in male and female rats.

Result : Survival was decreased for male rats. No effects were noted in rats in body weight gain. Non-neoplastic histopathological changes included forestomach lesions in male and female rats and nephropathy in male rats only.

Dose:	Observations
188 mg/kg bw/d:	NOEL; no effect
375 mg/kg bw/d:	LOEL; forestomach, lesions; mononuclear cell, leukemia (male); pancreatic acinar cell, adenoma (male); pituitary, adenoma (female); adrenal, pheochromocytoma (female)
750 mg/kg bw/d:	forestomach, lesions (male); adrenal, pheochromocytoma (male); benign and carcinoma (male)

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

19.05.2003

(87)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : oral feed
Exposure period : 2 years
Frequency of treatm. : 5 days/week
Post exposure period :
Doses : 0, 375 or 750 mg/kg bw
Result :
Control group : yes
Method : other
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

: The NTP report concluded that "there was equivocal evidence

5. Toxicity

Id 149-30-4

Date 18.06.2003

Remark : for carcinogenic activity" in female mice and no evidence for carcinogenic activity in male mice.
Result : Dose: Observations
375 mg/kg bw/d: liver, adenoma (female);
liver, carcinoma (female)
750 mg/kg bw/d: no effect.
Source : Bayer AG Leverkusen
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
16.05.2003 (88)

Species : mouse
Sex : male/female
Strain : other: Slc: ddY
Route of admin. : oral feed
Exposure period : 20 months
Frequency of treatm. : daily
Post exposure period :
Doses : 30, 120, 480 or 1920 ppm (males: 3.6, 14.7, 57.9 or 289.4 mg/kg bw day;
females: 3.6, 13.5, 58.9 or 284.0 mg/kg bw day)
Result :
Control group : yes
Method : other
Year : 1989
GLP : no data
Test substance : other TS: technical grade

Remark : see also chapter 5.4
Result : no significant increase in the tumour incidences
Source : Bayer AG Leverkusen
06.09.1994 (71)

Species : mouse
Sex : male/female
Strain : other: C57BL/6xC3H/Anf or C57BL/6xAKR hybrids
Route of admin. : other: gavage for 3 weeks and subsequently oral feed for 17 months
Exposure period : 18 months
Frequency of treatm. : daily
Post exposure period :
Doses : 100 mg/kg bw/day (gavage) and 323 ppm (oral feed: 50 mg/kg bw/day)
Result :
Control group : no data specified
Method :
Year : 1969
GLP : no data
Test substance : other TS: vehicle: 0.5 % gelatine

Remark : Rats were given 100 mg/kg bw/day in a suspension of the vehicle by gavage, beginning when the mice were 7 days of age until 4 weeks of age. After the mice were weaned at 4 weeks of age, the test substance was mixed directly with the diet (no vehicle was used) at a concentration of 323 ppm (50 mg/kg bw/day) for 17 months; 18 animals sex/strain/dose group.
Result : no significant increase in the incidence of tumors after oral administration of 2-mercaptobenzothiazole
Source : Bayer AG Leverkusen
01.09.1994 (89) (90)

Species : mouse
Sex : male/female

5. Toxicity

Id 149-30-4

Date 18.06.2003

Strain : other: B6C3F1 or B6AKF1 hybrids
Route of admin. : s.c.
Exposure period : see remark
Frequency of treatm. : single injection
Post exposure period : 17 months
Doses : 215 mg/kg bw
Result :
Control group : other: yes, concurrent vehicle and concurrent no treatment
Method : other: Carcinogenicity Test
Year : 1968
GLP : no data
Test substance : other TS: dissolved in 0.5 % gelantine

Remark : single s.c. injection in nape of neck at 28th day of age;
18 animals/sex/strain/dose and control group.

Result : No significant increase in the incidence of tumors was found.

Source : Bayer AG Leverkusen
01.09.1994

(89)

Species : other
Sex :
Strain :
Route of admin. :
Exposure period :
Frequency of treatm. :
Post exposure period :
Doses : 18.46 - 110.76 ug/ml
Result :
Control group :
Method : other: Cell transformation assay
Year : 1982
GLP : yes
Test substance : no data

Result : no increased number of transformed foci

Source : Bayer AG Leverkusen
06.09.1994

(81)

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : 10 weeks before mating, through gestation and lactation until sacrifice
Frequency of treatm. : ad libitum
Premating exposure period
Male : 10 weeks
Female : 10 weeks
Duration of test : approximately 88 days past weaning
No. of generation studies :
Doses : 0, 2500, 8750, or 15000 ppm (0, 179, 625, and 1071 mg/kg bw/d)
Control group : yes
NOAEL parental : < 2500 - ppm
NOAEL F1 offspring : < 2500 - ppm
NOAEL F2 offspring : < 2500 - ppm
Result : No observed adverse effects on reproductive parameters.

5. Toxicity

Id 149-30-4

Date 18.06.2003

Method : EPA OTS 798.4700
Year : 1991
GLP : yes
Test substance : other TS: MBT; purity = 98.1%

Remark : 2500, 8750, and 15000 ppm = 179, 625, and 1071 mg/kg bw/d
conversion number is 14

Result : Body weights were dose-dependently reduced for all treated F0 males and for mid- and high-exposure females. Body weights were reduced in the F1 pups from the mid- and high-exposure groups and in F2 pups from all dose levels beginning on Day 14 of lactation.

<u>Dose:</u>	<u>Observations</u>
2500 ppm:	F0: decr. bw (male) F1: decr. bw F2: decr. bw
8750 ppm:	F0: decr. bw; decr. food consumption, decr. kidney weight F1: decr. bw; decr. kidney weight (male); kidney, brown pigmentation; incr. liver weight; liver, hepatocellular hypertrophy F2: decr. bw
15000 ppm:	F0: decr. bw; decr. food consumption; decr. kidney weight F1: decr. bw; decr. kidney weight; kidney, brown pigmentation; incr. liver weight; liver, hepatocellular hypertrophy F2: decr. bw

Conclusion : There was no observation of adverse effects on reproductive parameters observed in this study.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

19.05.2003

(91)

Type : other
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : gestation and lactation and 35-days post-weaning
Frequency of treatm. : daily
Premating exposure period
 Male :
 Female :
Duration of test :
No. of generation :
studies
Doses : 5000, 10000, or 15000 ppm
Control group : yes
NOAEL parental : < 5000 - ppm
NOAEL F1 offspring : < 5000 - ppm
Method : other
Year : 1991
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : This was a rangefinding study.
5000, 10000, and 15000 ppm = 357, 714, and 1071 mg/kg bw/d
conversion number is 14
In the study report, there is reference to two different

5. Toxicity

Id 149-30-4

Date 18.06.2003

groups of F0 female rats. The first group, called Group 2, received MBT in the diet at a level of 15000 ppm throughout gestation and lactation. The F1 pups from these dams were exposed to 15000 ppm postweaning. The second group of F0 dams, called Group 3, received MBT in the diet at a level of 15000 ppm during gestation and the first week of lactation, 10000 ppm during the second week of lactation, and 5000 ppm during the third week of lactation. The F1 pups from these dams were exposed to 5000 ppm postweaning.

Result : Group 2 F0 dams: decr. bw; decr. food consumption
F1 pups: decr. bw
Group 3 F0 dams: decr. bw; decr. food consumption
F1 pups: decr. bw

Source : Bayer AG Leverkusen (92)
15.05.2003

Type : other: see Method
Species : rat
Sex : male/female
Strain : no data
Route of admin. : unspecified
Exposure period : see Method
Frequency of treatm. :
Premating exposure period
 Male :
 Female :
Duration of test :
No. of generation studies :
Doses :
Control group :
Method :
Year :
GLP :
Test substance : other TS: Captax, purity not noted

Method : Trial #1: 5-7 days before mating in males and at estrus state in females. Mating occurred during next estrus.
Trial #2: females exposed on day 4 and 11 of pregnancy after mating with untreated males.

Females sacrificed on 19th day of pregnancy.
Observations: number of yellow bodies (corpora lutea), number of live and dead fetuses, weight and length of fetuses.

Result : All accelerators tested had some effect on the development of the fetus.

Reliability : (4) not assignable
abstract only; translation from Russian (93)
27.04.2001

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : Day 6-15 of gestation
Frequency of treatm. : daily
Duration of test : up to Day 20 of gestation
Doses : 300, 1200, or 1800 mg/kg bw/d

5. Toxicity

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Date 18.06.2003

Control group : yes
NOAEL maternal tox. : = 300 - mg/kg bw
NOAEL teratogen. : = 1800 - mg/kg bw
Method : EPA OTS 798.4900
Year : 1991
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : The post-implantation loss was judged to be equivocal since it was not observed at 1200 mg/kg bw/d. There were no other indications that MBT was fetotoxic or teratogenic.

Result : Dose: Observation
300 mg/kg bw/d: PI loss.
1200 mg/kg bw/d: salivation (female);
urine staining (female);
dark red material around mouth (female)
1800 mg/kg bw/d: PI loss;
salivation (female);
urine staining (female);
dark red material around mouth (female);
decr. activity (female);
decr. bw (female);
decr. food consumption (female) Days 6-9.

Source : Bayer AG Leverkusen
Reliability : (1) valid without restriction
GLP Guideline study
Flag : Critical study for SIDS endpoint

16.05.2003

(94)

Species : rabbit
Sex : female
Strain : New Zealand white
Route of admin. : gavage
Exposure period : Day 6-18 of gestation
Frequency of treatm. : daily
Duration of test : up to Day 29 of gestation
Doses : 0, 50, 150, or 300 mg/kg bw/d
Control group : yes
NOAEL maternal tox. : = 300 - mg/kg bw
NOAEL teratogen. : = 300 - mg/kg bw
Result : No indication of fetotoxicity or teratogenicity compared to controls.
Method : EPA OTS 798.4900
Year : 1991
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : Quality Assurance Statement signed.

Result : No indication of fetotoxicity or teratogenicity compared to controls.
Maternal general toxicity: Slightly reduced body weight gain at 300 mg/kg (not statistically significant).

Dose: Observation
50 mg/kg bw/d: no effect.
150 mg/kg bw/d: NOEL; no effect.
300 mg/kg bw/d: incr. liver weight, (maternal);
decr. bw (maternal).

Reliability : (1) valid without restriction
GLP Guideline study
Flag : Critical study for SIDS endpoint

19.05.2003

(95)

5. Toxicity

Id 149-30-4

Date 18.06.2003

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : Day 6-15 of gestation
Frequency of treatm. : daily
Duration of test : up to Day 20 of gestation
Doses : 0, 300, 600, 1000, 1500, or 2200 mg/kg bw/d
Control group : yes
NOAEL maternal tox. : = 1000 - mg/kg bw
NOAEL teratogen. : = 2200 - mg/kg bw
Method : EPA OTS 798.4900
Year : 1991
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : Quality Assurance Statement signed.
This was a range-finding study. There was no observation of external abnormalities in fetuses.

Result :

<u>Dose:</u>	<u>Observations</u>
300 mg/kg bw/d:	no effect.
600 mg/kg bw/d:	no effect.
1000 mg/kg bw/d:	NOEL; no effect.
1500 mg/kg bw/d:	decr. bw (female)
2200 mg/kg bw/d:	decr. bw (female); mortality (female)

Source : Bayer AG Leverkusen
Reliability : (1) valid without restriction
GLP Guideline study

16.05.2003

(96)

Species : rabbit
Sex : female
Strain : New Zealand white
Route of admin. : gavage
Exposure period : Day 6-18 of gestation
Frequency of treatm. : daily
Duration of test : up to Day 29 of gestation
Doses : 150, 300, 600, 1000, or 1500 mg/kg bw/d
Control group : yes
NOAEL maternal tox. : < 150 - mg/kg bw
NOAEL teratogen. : = 300 - mg/kg bw
Method : other
Year : 1991
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : This was a range-finding study. There was no observation of treatment-induced external abnormalities in fetuses.

Result : 5) 1500 mg/kg bw/d:
mortality, F.

<u>Dose:</u>	<u>Observation</u>
150 mg/kg bw/d:	decr. bw (female); decr. viability (fetal); decr.bw (fetal).
300 mg/kg bw/d:	decr. bw (female); decr. viability (fetal); decr.bw (fetal).
600 mg/kg/bw d:	decr. bw (female); decr. viability (fetal); decr.bw (fetal).
1000 mg/kg bw/d:	mortality (female).
1500 mg/kg bw/d:	mortality (female).

5. Toxicity

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Source : Bayer AG Leverkusen
Reliability : (1) valid without restriction
GLP Guideline study
16.05.2003 (97)

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : i.p.
Exposure period : Days 1-15 of gestation
Frequency of treatm. :
Duration of test :
Doses : 200 mg/kg
Control group :
NOAEL maternal tox. : 200 - mg/kg bw
NOAEL teratogen. : 200 - mg/kg bw
Method : other: Hardin BD, Bond GP, Sikov MR, Andrew FD, Beliles RP, Niemeier RW. (1981) Scan. J. Work Environ. Hlth. 7(S4):66-75
Year :
GLP : no data
Test substance : other TS: 2-mercaptobenothiazole; purity not noted

27.04.2001 (98)

Species : rat
Sex : male/female
Strain : no data
Route of admin. : unspecified
Exposure period : see method
Frequency of treatm. :
Duration of test :
Doses : not specified
Control group :
Method :
Year :
GLP :
Test substance : other TS: Captax, purity not noted
Method : Trial #1: 5-7 days before mating in males and at estrus state in females. Mating occurred during next estrus.
Trial #2: females exposed on day 4 and 11 of pregnancy after mating with untreated males.
Females sacrificed on 19th day of pregnancy.
Observations: number of yellow bodies (corpora lutea), number of live and dead fetuses, weight and length of fetuses.
Result : All accelerators tested had some effect on the development of the fetus.
Reliability : (4) not assignable
abstract only; translation from Russian

27.04.2001 (93)

Species : other: chicken embryo
Sex :
Strain :
Route of admin. :
Exposure period :
Frequency of treatm. :
Duration of test :
Doses : 0.10, 0.50, 1.0, 1.5, 2.0 umoles/egg
Control group :
Method :

5. Toxicity

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Date 18.06.2003

Year :
GLP :
Test substance : other TS: Vulkacit Mercapto; technical grade

Method : Three day chicken embryos were selected by candling. 5ul of a solution of the test substance in acetone was injected onto the heart of the embryo (Korhonen et al. 1982. Scand. J. Work Environ. Hlth. 8:63). 5ul of acetone was used as a control substance. After 2 days the eggs were candled and dead embryos were discarded. Eggs were again candled every 2 or 3 days; those containing dead embryos were opened and checked for external malformations and the developmental stage. The incubation was terminated 11 days after injection and embryos inspected for survival and external malformations.

Result	Treatment (umoles/egg)	n=	early deaths	late deaths normal	late deaths malformed	malformed survivors	% affected
	0.10	9	0	0	0	1	11%
	0.50	30	0	0	0	5	17%
	1.0	40	7	0	1	7	38%
	1.5	30	6	0	0	6	40%
	2.0	30	4	0	0	9	43%

Median effective dose (ED50) = 2.0 umole/egg

27.04.2001

(99) (100)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

Remark : A mortality study of workers (2410 employees: 2160 men; 250 women) employed at a manufacturing chemicals plant for the rubber industries in the United Kingdom in the period 1955 - 1986 was performed. The eight hour time weighted average exposures to 2-mercaptobenzothiazole and its derivatives were estimated for different years and for each job and department title. Jobs attracted either zero exposure, very low (0 - 1 mg/m³), low (1 - 2.5 mg/m³), medium (2.5 - 6 mg/m³), or high exposure (6 - 20 mg/m³). The standardized mortality ratios (SMR) for all causes and the SMRs for mortality from cancer were not significantly different from 100. In this study estimated cumulative exposure to 2-mercaptobenzothiazole was not found to be a risk factor.

Source : Bayer AG Leverkusen
01.09.1994

(101)

Remark : Mortality trends for 1059 production workers at a rubber chemical plant in Nitro, West Virginia (USA) during 1955 - 1987 were examined to find whether they had increased mortality from cancer associated with exposure to 2-mercaptobenzothiazole. This chemical has been manufactured at the plant since 1935. Analyses were conducted on 2-mercaptobenzothiazole exposed employees by cumulative exposure and time since first exposure, and were also stratified by past assignment to p-aminobiphenyl-related departments; p-aminobiphenyl is a potent bladder carcinogen,

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that was used at the plant between 1935 and 1955. An excess of bladder cancer was seen in 2-mercaptobenzothiazole workers who also had job assignments with exposure to p-aminobiphenyl. In workers without a job assignment with exposure to p-aminobiphenyl, there were no associations between exposure to 2-mercaptobenzothiazole and increased rates of most malignant neoplasms. The standardized mortality ratio (SMR) for bladder cancer was raised, although there were too few deaths to evaluate trends exposure category. There were no deaths from bladder cancer among 2-mercaptobenzothiazole workers hired after the end of p-aminobiphenyl use at the plant although only 0.03 deaths were expected.

Source : Bayer AG Leverkusen (102)
02.09.1994

5.11 ADDITIONAL REMARKS

Type : Chemobiokinetics general studies

Remark : 72 % radioactivity excreted in urine and 4 % in feces in 96 hr.
Male and female Fischer 344 rats were dosed orally with 0.592 or 55.5 mg/kg of ¹⁴C-labelled MBT, then sacrificed at 8, 24, 72, or 96 hr post-dosing.

Source : Bayer AG Leverkusen (103)
06.11.2000

Type : Chemobiokinetics general studies

Remark : Male and female rats and female guinea pigs were topically exposed to ¹⁴C-MBT at approximately 36.1% ug/animal. A separate set of rats were also dosed orally for 14 days with unlabelled MBT at 0.51 mg/kg/day prior to a single dose with 0.503 mg/kg of radiolabelled material. A third set of rats received radiolabelled MBT iv at a dosage of 0.602 mg/kg. Urine excretion of the absorbed dose was > 91 %.

Source : Bayer AG Leverkusen (104)
02.06.1994

Type : Neurotoxicity

Remark : Decreased motor activity was noted.
This study was a rangefinding study. Male and female Sprague-Dawley rats were given MBT by gavage in a corn oil vehicle at dosage levels of 0 or 2750 mg/kg and then observed for 24 hr in a motor activity assessment.

Source : Bayer AG Leverkusen (105)
03.11.2000

Type : Neurotoxicity

Remark : Male and female Sprague-Dawley rats were dosed once by gavage with MBT in a corn oil vehicle at levels of 0, 500, 1250, or 2750 mg/kg bw and then observed for 14 days. Motor activity testing and a functional observational battery were performed.

Based on the findings, it was concluded that the effects seen may be related to an acute, non-specific toxicity

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- Source**
03.11.2000
- without apparent neurotoxicity.
: Bayer AG Leverkusen (106)
- Type**
: Neurotoxicity
- Remark**
: 5000 ppm: NOEL; no effect.
In a three-month study, MBT was administered to Sprague-Dawley rats in the diet at levels of 0, 5000, 15000, or 25000 ppm. [5000, 15000, and 25000 ppm = 357, 2500, and 1786 mg/kg bw, conversion number is 14.] Motor activity, functional observational battery, and gross and microscopic evaluations were performed.
- Source**
03.11.2000
- : Bayer AG Leverkusen (107)
- Type**
: other
- Remark**
: Revision of chapter 5 (without inquiry): September 94
- Source**
06.09.1994
- : Bayer AG Leverkusen
- Type**
: other: DNA binding study
- Remark**
: Male and female Fischer 344 rats received a single dose of 375 mg [¹⁴C]2-mercaptobenzothiazole/kg bw by gavage; after 8 hours rats were killed, DNA was extracted from liver, adrenals, pituitary gland, pancreas and bone marrow and the amount of DNA associated radioactivity was determined. 2-mercaptobenzothiazole does not significantly bind to DNA from any of the tissues examined. The covalent binding index (CBI) for liver was approximately 1 to 3. The covalent binding indices for the other tissues were below 1. Strong hepatocarcinogens such as dimethylnitrosamine and aflatoxin have CBI values ranging from 6000 to greater than 20000.
- Source**
01.09.1994
- : Bayer AG Leverkusen (108)

6. Analyt. Meth. for Detection and Identification

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6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

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7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8. Meas. Nec. to Prot. Man, Animals, Environment

Id 149-30-4
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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

I U C L I D

Data Set

Existing Chemical : ID: 155-04-4
CAS No. : 155-04-4
EINECS Name : zinc di(benzothiazol-2-yl) disulphide
EC No. : 205-840-3
Molecular Formula : C7H5NS2.1/2Zn

Producer related part
Company : Bayer Corporation
Creation date : 15.07.1999

Substance related part
Company : Bayer Corporation
Creation date : 15.07.1999

Status :
Memo : American Chemistry Council, Rubber and Plastic Additives Panel,
Benzothiazole-based Thiazoles Category

Printing date : 18.06.2003
Revision date :
Date of last update : 18.06.2003

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Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 155-04-4

Date 18.06.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation
Name : American Chemistry Council, Rubber and Plastic Additives Panel (RAPA)
Contact person :
Date :
Street : 1300 Wilson Boulevard
Town : VA 22209 Arlington
Country : United States
Phone : 703-741-5600
Telefax : 703-741-6091

16.05.2003

Type : cooperating company
Name : Bayer Polymers LLC (a wholly -owned subsidiary of Bayer Corporation)
Contact person :
Date :
Street : 100 Bayer Road, Building #5
Town : PA 15205-9741 Pittsburgh
Country : United States

18.06.2003

Type : cooperating company
Name : Crompton Corporation
Contact person :
Date :
Street : Benson Road
Town : 06749 Middlebury, CT
Country : United States

18.06.2003

Type : cooperating company
Name : Flexsys America, L.P.
Contact person :
Date :
Street : 260 Springside Drive
Town : OH 44333-0444 Akron
Country : United States

18.06.2003

Type : cooperating company
Name : Noveon, Inc.
Contact person :
Date :
Street : 9911 Brecksville Road
Town : 44141-3247 Cleveland, OH
Country : United States

18.06.2003

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1. General Information

Id 155-04-4
Date 18.06.2003

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name : 2(3H)-benzothiazolethione, zinc salt
Smiles Code : [Zn](Sc2nc1cccc1s2)Sc4nc3cccc3s4
Molecular formula : C14-H8-N2-S4-Zn
Molecular weight : 397.85
Petrol class :

14.04.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : solid
Purity : - 97 % w/w
Colour :
Odour :

14.04.2003

(1)

Purity type : typical for marketed substance
Substance type : organic
Physical status : solid
Purity : 86 - 98 % w/w
Colour : Off-white to pale yellow solid
Odour :

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(2)

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2-benzothiazole, zinc salt

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2-mercaptobenzothiazole, zinc salt

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ZMBT

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Zinc MBT

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Bantex®

14.04.2003

Perkacit® ZMBT

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1. General Information

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Vulcafor® ZMBT

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Vulkacit® ZM

14.04.2003

Zetax®

14.04.2003

1.3 IMPURITIES

Purity :
CAS-No : 149-30-4
EC-No : 205-736-8
EINECS-Name : benzothiazole-2-thiol
Molecular formula : C7H5NS2
Value : 2 - 14 % w/w

14.04.2003

Purity :
CAS-No :
EC-No :
EINECS-Name : inorganics (NaCl, NaSO4)
Molecular formula :
Value : <= .5- % w/w

13.10.1999

Purity :
CAS-No : 7732-18-5
EC-No : 231-791-2
EINECS-Name : water
Molecular formula :
Value : <= .3- % w/w

13.10.1999

1.4 ADDITIVES

Purity type :
CAS-No :
EC-No :
EINECS-Name : emulgator
Molecular formula :
Value : 0 - .5 % w/w
Function of additive :

13.10.1999

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1. General Information

Id 155-04-4
Date 18.06.2003

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : type
Category : Non dispersive use

13.10.1999

Type of use : industrial
Category : Polymers industry

13.10.1999

Type of use : use
Category : Vulcanizing agents

13.10.1999

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

Type : TSCA
Additional information :

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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. Physico-Chemical Data

Id 155-04-4

Date 18.06.2003

2.1 MELTING POINT

Value : 337 - °C
Decomposition : no, at - °C
Sublimation : no
Method : other: Instrumental - Differential Scanning Calorimeter, 2000
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : 2.0 grams of sample analyzed under nitrogen atmosphere.
DSC heating rate of 10°C/minute
The free MBT (2-mercaptobenzothiazole) portion of the test substance melts at 176.6°C.

Reliability : (1) valid without restriction
GLP study

Flag : Critical study for SIDS endpoint

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(3)

2.2 BOILING POINT

Value : 361.8 - °C at 38.66 hPa
Decomposition : yes
Method : other: Instrumental - Differential Scanning Calorimeter, 2000
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : Thermal decomposition occurs before boiling
[Pressure = 29 mm Hg (38.66 hPa)]

Reliability : (1) valid without restriction
GLP study

Flag : Critical study for SIDS endpoint

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(3)

2.3 DENSITY

Type : density
Value : ca. 1.7 - g/cm³ at 20 °C
Method : other: Density of solids by displacement of liquid
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

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(4)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .0000000264 - hPa at 25 °C
Decomposition :
Method : other (calculated): MPBPWIN v1.40
Year :
GLP : no

2. Physico-Chemical Data

Id 155-04-4

Date 18.06.2003

Test substance : other TS: molecular structure
Remark : 1.98E-008 mm Hg
Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
14.04.2003

(5)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : 5.02 - at 25 °C
pH value : -
Method : other (calculated): KOWWIN v1.66
Year :
GLP : no
Test substance : other TS: molecular structure
Remark : Estimation method based on molecular structure fragments and measured melting point and water solubility
Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
14.04.2003

(5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : 90.9 - mg/l at 20 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : slightly soluble (0.1-100 mg/L)
Stable :
Deg. product :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Compares favorably with the measured water solubility of 2-mercaptobenzothiazole (MBT) of 118 mg/l @ 25°C
Source : Bayer AG Leverkusen
Flag : Critical study for SIDS endpoint
14.04.2003

(1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2. Physico-Chemical Data

Id 155-04-4

Date 18.06.2003

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

Memo : Henry's Law constant

Method : HENRYWIN v3.10, EPIWIN

Remark : Calculated at 25°C using measured melting point and solubility

Result : 1.51E-017 atm-m³/mole

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(6) (5)

3. Environmental Fate and Pathways

Id 155-04-4

Date 18.06.2003

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 :
Rate constant : ca. .0000000000902585 cm³/(molecule*sec)
Degradation : ca. 50 - % after 1.4 hour(s)
Deg. product :
Method : other (calculated):AopWin v1.88 Estimations Program
Year : 1999
GLP :
Test substance : other TS: chemical structure

Remark : Rapid atmospheric degradation of test substance in vapor phase by reaction with photochemically produced hydroxyl radicals. Particulate phase test substance may be physically removed from air by both wet and dry deposition. If released to air, test substance is expected to exist in both vapor and particulate phases.

Reliability : (2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint
14.04.2003 (7)

3.1.2 STABILITY IN WATER

Type : abiotic
Degradation : - 15 % after 7 day(s) at pH 7 and °C
Deg. product :
Method : other: Monsanto protocol
Year :
GLP : yes
Test substance : **other TS: 2-mercaptobenzothiazole (CAS# 149-30-4)**

Remark : Zinc MBT will dissociate to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thiozoles category of chemicals.

Reliability : (1) valid without restriction
GLP study
18.06.2003 (8)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : volatility
Media : water - air
Method : other: Estimation Method, 1990
Year :
Remark : Model river = 1 m deep flowing at 1 m/sec and wind velocity of 3 m/sec.

3. Environmental Fate and Pathways

Id 155-04-4

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Model lake = 1 m deep flowing at 0.05 m/sec and wind velocity of 0.5 m/sec.
Result : Volatilization half-life from model river: 7.734E+013 hours
Volatilization half-life from model lake: 8.437E+014 hours
Reliability : (2) valid with restrictions
Data from Handbook or collection of data
14.04.2003 (9)

Type : fugacity model level III
Media : other: Air-water-soil-sediment
Method : other: EPISUITE/EPIWIN v3.10
Year :

Remark : Modeling was performed using equal releases (1000 kg/hr) and equal distribution to all compartments.

Result : Media Distribution (%) Half-life (hrs) Emissions (kg/hr)
Air 1.73E-010 2.84 1000
Water 14.5 900 1000
Soil 66.6 900 1000
Sediment 18.9 3.6E+003 0

Reliability : Persistence time estimated to be 1.23E+003 hours
(2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint
14.04.2003 (5)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 23.8 mg/l related to Test substance related to
Contact time :
Degradation : < - 1 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Deg. product :
Method : EPA OTS 796.3100
Year : 1989
GLP : yes
Test substance : **other TS: 2-mercaptobenzothiazole, purity = 98%**
Method : Gledhill method listed in U.S. TSCA regulations 40 CFR Ch 1 subpart D paragraph 796.3100
Remark : Zinc MBT will dissociate to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thiozoles category of chemicals.
Reliability : (1) valid without restriction
GLP Guideline study
18.06.2003

3.6 BOD5, COD OR BOD5/COD RATIO

BOD5
Method : other
Year :
Concentration : related to

3. Environmental Fate and Pathways

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Date 18.06.2003

BOD5 : 0 mg/l
GLP :
Remark : no degradation
Source : Bayer AG Leverkusen
14.04.2003

(1)

3.7 BIOACCUMULATION

Species : other
Exposure period : at °C
Concentration :
BCF : 1453 -
Elimination :
Method : other: BCFWIN v2.14
Year :
GLP : no
Test substance : other TS: molecular structure

Remark : Calculation using measured melt point and water solubility
Result : Log BCF = 3.162
Reliability : (2) valid with restrictions
Accepted calculation method

14.04.2003

(5)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 155-04-4

Date 18.06.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : field observation
Species : Leuciscus idus (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
LC0 : 10 -
LC100 : 50 -
Limit test :
Analytical monitoring : no
Method : other: Bestimmung der akuten Wirkung von Stoffen auf Fische. Arbeitskreis "Fischtest" im Hauptausschuss "Detergentien" (15.10.73)
Year : 1975
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : direct weight; closed system
Source : Bayer AG Leverkusen
Reliability : (2) valid with restrictions
Guideline study; lack of method detail.
Flag : Critical study for SIDS endpoint
14.04.2003 (1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : 1.9 -
EC50 : 2.9 -
Method : other: "Protocol for Conducting a Static Acute Toxicity Test with Daphnia magna Following FIFRA Guideline 72", SLI Protocol #010190/FIFRA 72-2 DM SA and protocol amendment #1 dated 9 January 1992
Year : 1992
GLP : yes
Test substance : **other TS: 100 % 2-Mercaptobenzothiazole (CAS# 149-30-4)**

Remark : Zinc MBT is similar in toxicity to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thizoles category of chemicals.
Reliability : (1) valid without restriction
GLP Guideline study
14.05.2003

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : biomass
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : .25 -
Limit test :
Analytical monitoring : no
Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year : 1984
GLP : no data

4. Ecotoxicity

Id 155-04-4

Date 18.06.2003

Test substance : other TS: 100 % 2-Mercaptobenzothiazole (CAS# 149-30-4)

Remark : C.I. 0.06-0.98 mg/l; in vivo chlorophyll results - 24 and 48h-EC50 >0.3<0.6 mg/l, 96h-EC50: 0.23 mg/l
Zinc MBT is similar in toxicity to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thizoles category of chemicals.

Test condition : temp 24 degrees Celsius; 4000 lux; Algal Assay Media; init. inoc. 10000 cells/ml; "cool" white lights

Reliability : (1) valid without restriction
Guideline study

14.05.2003 (10)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic

Species : activated sludge

Exposure period : 3 hour(s)

Unit : mg/l

EC50 : 1220 -

EC05 : 70 -

Analytical monitoring : no

Method : ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"

Year : 1990

GLP : yes

Test substance : as prescribed by 1.1 - 1.4

Remark : Direct weighing, nominal concentration, high bacteria density as described in ISO 8192

Source : Bayer AG Leverkusen

Reliability : (1) valid without restriction
GLP Guideline study

14.04.2003 (1)

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. Toxicity

Id 155-04-4

Date 18.06.2003

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : 5505 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals :
Vehicle :
Doses :
Method : EPA OPP 81-1
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Result : LD50
5505 mg/kg bw (combined)
5735 mg/kg bw (males)
5221 mg/kg bw (females)

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint

14.05.2003

(11)

Type : LD50
Value : = 7500 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 20
Vehicle : other: corn oil
Doses : 5000, 6310, 7940 or 10,000 mg/kg bw
Method : other: Single Oral Dose, Younger Laboratories Protocol, 1973
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Four groups of male and female rats (5/sex/dose level) were fed a single oral dose of the test article as a 20% suspension in corn oil via oral gavage. Male rats had initial average body weights of 210-245 grams; females were 220-240 grams. Clinical signs of toxicity included reduced activity and appetite for 1-3 days for survivors, and increasing weakness, collapse and death for decedents in 1-2 days with most deaths occurring within 2 days. Gross autopsy findings on decedents were liver hyperemia, hemorrhagic areas of the lungs and gastrointestinal inflammation. Survivors were sacrificed after a fourteen day observation period. All viscera appeared normal in these animals.

<u>Dose mg/kg</u>	<u>Mortalities-</u>		
	Male	Female	Combined
5000	0/3	0/2	0/5
6310	1/2	0/3	1/5
7940	1/3	2/2	3/5
10000	2/2	3/3	5/5

5. Toxicity

Id 155-04-4

Date 18.06.2003

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

Flag : Critical study for SIDS endpoint (12)
14.05.2003

Type : LD50
Value : > 10000 - mg/kg bw
Species : rat
Strain : Wistar
Sex : male/female
Number of animals : 20
Vehicle : other: propylene glycol
Doses :
Method :
Year :
GLP : no data
Test substance : other TS: Vulcafor ZMBT; purity not noted

Method : The test material was given as a 33% (w/v) suspension in propylene glycol to groups of 10 males and 10 females in a single dose of 30 ml/kg bw (10g test material/kg bw). The rats received feed and water ad libitum during the 14 day observation period. The rats were observed for intoxication and mortality. All animals were necropsied.

Remark : mortality: 4/20 died. Within a few minutes of dosing, all rats showed sluggishness, followed by loss of consciousness. Two males and two females died between 2 and 15 hours after treatment. After 24 hours, the survivors recovered and looked healthy during the 14 day observation period. Macroscopic examination of the survivors did not reveal treatment-related gross alterations.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint (13)
16.04.2003

Type : LD50
Value : > 5000 - mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other
Year :
GLP : no data
Test substance : other TS: commercial grade

Remark : mortality: 0/20 (14) (15)
25.04.2001

5.1.2 ACUTE INHALATION TOXICITY

5. Toxicity

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Date 18.06.2003

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 : 10
Vehicle : physiol. saline
Doses : 2000 mg/kg
Method : EPA OPP 81-2
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : All animals survived to study termination on day 15. Slight erythema was noted at application site. Mean body weight decreased in both sexes from study days 1-4, but increased for the remainder of the study. The small intestines of two males and one female appeared distended at gross necropsy; all other animals were normal.

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint
14.05.2003

(16)

Type : LD50
Value : > 7940 - mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 2
Vehicle : other: corn oil
Doses : 7940 mg/kg bw
Method : other: Single Dermal Dose, Younger Laboratory Protocol, 1974
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Signs of intoxication were reduced appetite and activity that lasted for two to four days. After a fourteen day observation period, the animals were sacrificed. All viscera appeared normal in both animals.

<u>Dose mg/kg</u>	<u>Mortalities</u>		
	Male	Female	Combined
7940	0/1	0/1	0/2

Test condition : The test substance was applied to the shaved skin of one male and one female rabbit as a 40% suspension in corn oil. The male rabbit weighed 2.1 kg, and the female weighed 2.0 kg. The test material was held in place by means of an occlusive wrap of latex rubber and secured by bandaging and elastic tape. The occlusive wrap was removed after 24 hours and the excess material was wiped from the test animal. Clinical observations were made three times during the first eight hours after dosing, and twice daily thereafter until sacrifice.

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

Flag : Critical study for SIDS endpoint
16.04.2003

(17)

5. Toxicity

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5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : other: approx. LD50
Value : 200 - 300 mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Route of admin. : i.p.
Exposure time :
Method : no data
Year :
GLP : no data
Test substance : no data

Source : Bayer AG Leverkusen
21.09.1994

(18)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : 50 %
Exposure :
Exposure time :
Number of animals : 6
Vehicle : physiol. saline
PDII : .04
Result : slightly irritating
Classification : not irritating
Method : EPA OPP 81-5
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : Slight dermal irritation in one of three test animals.
Test substance : Concentration: 50% (0.5 g in 0.5 ml saline)
Reliability : (1) valid without restriction
GLP Guideline study

16.04.2003

(19)

Species : rabbit
Concentration : .5 g
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII : 0
Result : not irritating
Classification : not irritating
Method : other: Draize, J.H., Woodard, G., and Calvery, H.O., 1944 and A.T.S., 1973
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : 0.5 grams of the test substance, as a finely ground powder moistened with water, was applied to the shaved dorsal areas of six albino rabbits. The test material was applied to the skin under 1" square gauze patches and held in

5. Toxicity

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Date 18.06.2003

contact with the skin by means of an occlusive wrap of latex rubber secured by bandaging and elastic tape. The occlusive wrap and gauze patches were removed after 24 hours. Dermal irritation was scored by the Draize Method, and results were recorded 24, 48, 72 and 168 hours after topical application.

Result : The Primary Irritation Index was calculated by averaging the mean scores at 24 and 72 hours. The Primary Irritation Index was found to be 0.0 on a scale of 0.0-8.0. All animals scored zero at each observation period.

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

16.04.2003 (20)

Species : rabbit
Concentration : 50 %
Exposure :
Exposure time :
Number of animals : 6
Vehicle : physiol. saline
PDII : .04
Result : not irritating
Classification : not irritating
Method : other: 24 hour exposure, 7 day observation
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Scores in accordance with Federal Hazardous Substances Act, 21 CFR, Part 191.12 (1964)

Test substance : Concentration: 50% (0.5 g in 0.5 ml saline)

Reliability : (2) valid with restrictions
age of study, lack of method detail

16.04.2003 (1)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : not irritating
Classification :
Method : other: 24 hours exposure; 7-d observation period
Year :
GLP : no data
Test substance : other TS: no data

Remark : scores in according to the method of Draize

Source : Bayer AG Leverkusen

14.04.2003 (21)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : 74.1 %
Dose :
Exposure time : 24 hour(s)
Comment :
Number of animals : 6

5. Toxicity

Id 155-04-4

Date 18.06.2003

Vehicle :
Result : slightly irritating
Classification : not irritating
Method : EPA OPP 81-4
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : An application of 74.06% of the test substance to the eyes of rabbits caused conjunctival redness, chemosis and discharge.

Reliability : (1) valid without restriction
GLP Guideline study

14.05.2003

(22)

Species : rabbit
Concentration : 100 mg
Dose :
Exposure time : 24 hour(s)
Comment : not rinsed
Number of animals : 6
Vehicle : none
Result : slightly irritating
Classification : not irritating
Method : other: 100 mg was placed into the conjunctival sac of 6 rabbits; 7-d observation period
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : 100 mg of the test substance, as a finely ground powder, was applied to one eye of six albino rabbits. The other eye was not treated and served as a control. The cornea, iris and conjunctiva were examined immediately after treatment, and then at intervals of 10 minutes, 1 hour, and then at 24, 48, 72 and 168 hours.

Result : The Draize Method was used for scoring eye irritation.

Exposure time	Mean score (x/110)
24 hours	7.3
48 hours	5.3
72 hours	0.0
168 hours	0.0

PDII = 1.7/110.0

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

14.05.2003

(23)

Species : rabbit
Concentration : 100 mg
Dose :
Exposure time : 24 hour(s)
Comment :
Number of animals : 6
Vehicle : none
Result : not irritating
Classification : not irritating
Method : other: FDA, 1963
Year :
GLP : no data
Test substance : other TS: no data

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Remark : 100 mg of the test substance, as a finely ground powder, was applied to one eye of six albino rabbits. The other eye was not treated and served as a control. Scoring for irritation was in accordance with the FDA scoring scale, Fed. Reg. 28 (119), 5582, 1963.

Reliability : (2) valid with restrictions
lack of method detail

14.05.2003 (24)

5.3 SENSITIZATION

Type : Mouse local lymphnode assay
Species : mouse
Number of animals :
Vehicle : other: Acetone-olive oil
Result : sensitizing
Classification :
Method : other: Local Lymph Node Assay, 1999
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : A modified Local Lymph Node Assay (LLNA) with ex vivo tritium thymidine (3H-TdR) labeling of the proliferating lymph node cells was used for determination of the allergic potential of chemicals used in the production of latex for medical gloves. 15 different chemicals with known or suspected capability to induce contact hypersensitivity reactions in humans were tested. 14 out of 15 chemicals tested as sensitizers.

Result : ZMBT: The EC3 value (effective concentration inducing a 3-fold increase in 3H-thymidine incorporation in the harvested lymph node cells of the treated animals compared to vehicle-treated animals) was 30.3%, indicating a weak response.

Conclusion : The authors concluded that ZMBT would be the rubber accelerator of choice from the benzothiazole-based thiazoles category for use in exam gloves to minimize the potential for contact hypersensitivity reactions.

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

15.04.2003 (25)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals : 10
Vehicle : physiol. saline
Result : not sensitizing
Classification : not sensitizing
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : No erythema noted in test or naïve control animals at 26 and 48 hours after challenge application.

Test condition : Dose: 0.5 g
Vehicle: Physiological saline, 0.5 ml

Reliability : (1) valid without restriction

16.04.2003 (26)

Type : Patch-Test
Species : human
Concentration : 1st: Challenge 1 % semioclusive

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2nd.
3rd.
Number of animals : 17
Vehicle : petrolatum
Result : sensitizing
Classification : sensitizing
Method : other: Human Patch test
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : The test substance, as a 1% preparation in petrolatum, was applied to the skin of 17 human volunteers who had previously tested positive to MBT (2-mercaptobenzothiazole). Fifteen out of seventeen test subjects also responded positively to ZMBT.

14.04.2003 (27)

Type : Patch-Test
Species : human
Number of animals :
Vehicle :
Result :
Classification :
Method : other
Year :
GLP : no data
Test substance : other TS: 1 % in Eucerin anhydric

Remark : result: 2/5 patients with a rubber eczema were positive with Zn-MBT among other chemicals tested.

Source : Bayer AG Leverkusen
18.06.2003 (28)

5.4 REPEATED DOSE TOXICITY

Type : Chronic
Species : mouse
Sex :
Strain : other: B6C3F1 and B6AKF1
Route of admin. : other: gavage (days 7-28 of age) and in the diet (after 28 days of age)
Exposure period : 18 months
Frequency of treatm. : daily
Post exposure period :
Doses : 1000 mg/kg (gavage) 2600 ppm (diet)
Control group :
NOAEL : 1000 - mg/kg bw
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : There were no significant adverse affects were seen that could be attributed to the test substance, Zn-MBT.

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

Flag : Critical study for SIDS endpoint
14.05.2003 (29)

5. Toxicity

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5.5 GENETIC TOXICITY 'IN VITRO'

Type	: Bacterial gene mutation assay
System of testing	: S. typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Test concentration	: 0.1, 1.0, 10, 100 or 500 ug/plate (duplicate)
Cycotoxic concentr.	: With metabolic activation: 500 ug/plate, TA-1538 only; Without metabolic activation: 500 ug/plate, TA-1538 only
Metabolic activation	: with and without
Result	: negative
Method	: other: Ames Mutagenicity Plate Test (Overlay Method) 1975
Year	:
GLP	: no data
Test substance	: as prescribed by 1.1 - 1.4
Remark	: The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The Salmonella typhimurium strains used for this experiment were obtained from Dr. Bruce Ames. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. Chemicals used as positive controls for the non-activation assays were methylnitrosoguanidine (MNNG), 2-nitrofluorene (NF) and quinacrine mustard (QM). Positive control chemicals used for the activation assays were 2-anthramine (ANTH), 2-acetylaminofluorene (AAF) and 8-aminoquinoline (AMQ). Dimethylsulfoxide (DMSO) at 50 ug/plate was used as the solvent and the solvent control.
Result	: The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.
Reliability	: (2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag	: Critical study for SIDS endpoint
14.05.2003	(30)
Type	: Gene mutation in Saccharomyces cerevisiae
System of testing	: strain D4
Test concentration	: 0.1, 1.0, 10, 100 and 500 micrograms/plate.
Cycotoxic concentr.	: With metabolic activation: 500 micrograms/plate; Without metabolic activation. 500 micrograms/plate
Metabolic activation	: with and without
Result	: negative
Method	: other: Ames Mutagenicity Plate Test (Overlay Method) 1975
Year	:
GLP	: no data
Test substance	: as prescribed by 1.1 - 1.4
Remark	: The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. The chemical used as the positive control for the non-activation assay was methylnitrosoguanidine (MNNG) at 10 ug/plate. Positive control chemical used for the activation assay was DMNA at 100 micromoles/plate. Dimethylsulfoxide (DMSO) at 50 ul/plate was used as the solvent and the solvent control.

5. Toxicity

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- Result** : The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.
- Reliability** : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
- Flag** : Critical study for SIDS endpoint
15.04.2003 (30)
- Type** : Bacterial gene mutation assay
System of testing : S. typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Test concentration : up to 3000 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result :
Method : other: no data
Year :
GLP : no data
Test substance : no data
- Remark** : result: weakly positive (+ S9-mix)
Source : Bayer AG Leverkusen
22.09.1994 (31)
- Type** : Bacterial gene mutation assay
System of testing : S. typhimurium TA 98, TA 100, TA 1535, TA 1537
Test concentration : up to 3000 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other: Ames Mutagenicity Plate Test (Overlay Method) 1975
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
15.04.2003 (32)
- Type** : Bacterial gene mutation assay
System of testing : S. typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Test concentration :
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other
Year :
GLP :
Test substance : no data
- Remark** : substance was not toxic for the test strains in higher concentrations
Source : Bayer AG Leverkusen
21.09.1994 (33)
- Type** : Ames test
System of testing : S. typhimurium
Test concentration :
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Test substance :
30.10.2000 (34)

5. Toxicity

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5.6 GENETIC TOXICITY 'IN VIVO'

Type	: other: Mammalian Chromosome Aberration Test
Species	: mouse
Sex	: male/female
Strain	: Swiss
Route of admin.	: i.p.
Exposure period	: 36 hours
Doses	: 0, 480, 960 or 1920 ug/20 g bw
Result	: negative
Method	: OECD Guide-line 475 "Genetic Toxicology: In vivo Mammalian Bone Marrow Cytogenetic Test - Chromosomal Analysis"
Year	: 1997
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Result	: The results indicated a lack of incidence of chromosomal abnormalities in both the test compound and vehicle groups. Significant chromosomal abnormalities, such as gaps, breaks and translocations were observed in the positive control group. The test article failed to induce structural chromosomal aberrations in mouse bone marrow cells at any of the doses tested.
Test condition	: The induction of chromosomal aberrations by the rubber accelerator ZMBT was studied in Swiss albino mice. Three groups of four mice received the test substance at doses of 1920, 960 or 480 ug/20g body weight. The remaining groups of four mice received the vehicle (cotton seed oil) or the positive control chemical methyl methanesulfonate. The animals were given a single dose of the test substance and control substances by i.p. injection. Colchicine, at 20 ug/animal, was administered 90 minutes before sacrifice. All test animals were sacrificed after 36 hours by cervical dislocation. Bone marrow preparations were made, stained with Giesma stain, and examined for chromosomal abnormalities.
Reliability	: (1) valid without restriction GLP Guideline study
Flag	: Critical study for SIDS endpoint
15.04.2003	(35)

5.7 CARCINOGENICITY

Species	: mouse
Sex	: male/female
Strain	: other: B6C3F1 and B6AKF1
Route of admin.	: other: gavage (days 7-28 of age) and in the diet (after 28 days of age)
Exposure period	: 18 months
Frequency of treatm.	: daily
Post exposure period	: no
Doses	: 1000 mg/kg (gavage) 2600 ppm (diet)
Result	: negative
Control group	: yes, concurrent vehicle
Method	: other
Year	:
GLP	: no data
Test substance	: as prescribed by 1.1 - 1.4
Method	: In a National Cancer Institute study, 18 virgin male and 18 virgin female mice from two hybrid strains were dosed with the test substance. A group of 36 mice received a daily oral intubation dose of the test article administered from the 7th to 28th days of age, and then daily in their feed mix thereafter.

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Result	:	There were no statistically significant increases in tumor incidences observed and no significant adverse affects were seen that could be attributed to the test substance, Zn-MBT.
Reliability	:	All compounds administered orally as positive controls were carcinogenic. (2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
15.04.2003		(36) (29)
Species	:	mouse
Sex	:	male/female
Strain	:	other: B6C3F1 and B6AKF1
Route of admin.	:	other: a single s.c. injection at 28th day of age
Exposure period	:	
Frequency of treatm.	:	once
Post exposure period	:	18 months
Doses	:	1000 mg/kg
Result	:	negative
Control group	:	yes, concurrent vehicle
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	In a National Cancer Institute study, 18 virgin male and 18 virgin female mice from two hybrid strains were dosed with the test substance. A group of 36 mice received a single subcutaneous injection (1000 mg/kg as 0.05 ml of suspension) administered in the nape of the neck at the 28th day of age, with no exposure to the test substance thereafter.
Remark	:	Study was undertaken to determine the carcinogenic potential of 130 chemicals that had been used in the formulations of insecticides, herbicides and fungicides.
Result	:	There were no statistically significant increases in tumor incidences observed and no significant adverse affects were seen that could be attributed to the test substance, Zn-MBT. Two positive controls (urethane, ethyleneimine) administered subcutaneously had carcinogenic activity.
Source	:	Bayer AG Leverkusen
Reliability	:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment, however, the reliance on a single subcutaneous injection as adequate for this study is questionable.
15.04.2003		(29)

5.8.1 TOXICITY TO FERTILITY

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	other: CrI: CD COBS BR
Route of admin.	:	oral feed
Exposure period	:	
Frequency of treatm.	:	
Premating exposure period	:	
Male	:	
Female	:	
Duration of test	:	
No. of generation studies	:	
Doses	:	0, 2500, 8750, 15000 ppm (0, 194, 695, 1195 mg/kg/day)
Control group	:	

5. Toxicity

Id 155-04-4

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Method : EPA OPPTS 870.3800
Year :
GLP :
Test substance : **other TS: 2-mercaptobenzothiazole (CAS# 149-30-4)**

Remark : Zinc MBT is similar in toxicity to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thizoles category of chemicals.

Result : Reproductive/systemic NOEL = 2500 ppm (194 mg/kg/day), LOEL = 8750 ppm (695 mg/kg/day) based on decrease in body weight.

14.05.2003 (37)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : Gestation days 6 -15
Frequency of treatm. : daily
Duration of test :
Doses : 0, 300, 1200, 1800 mg/kg/day
Control group : yes
NOAEL maternal tox. : 300 - mg/kg bw
NOAEL teratogen. : 1200 - mg/kg bw
Method : EPA OPPTS 870.3700
Year :
GLP :
Test substance : **other TS: 2-mercaptobenzothiazole (CAS# 149-30-4)**

Remark : Zinc MBT is similar in toxicity to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thizoles category of chemicals.

Result : The LOEL for maternal toxicity was 1200 mg/kg/day due to hair loss, increased salivation and urine staining. The LOEL for developmental toxicity was 1800 mg/kg/day due to greater post-implantation loss.

Reliability : (1) valid without restriction

14.05.2003 (38)

Species : other: Chicken embryos
Sex : male/female
Strain : other: White Leghorn
Route of admin. : other: Injection into egg air chamber
Exposure period : 11 days (Day 3 - Day 14)
Frequency of treatm. : Once on Day 3
Duration of test :
Doses : 0-1.0 umoles/egg
Control group : yes, concurrent vehicle
Result : No effect on embryos. NOEL teratogenicity : 1.0 umoles/egg
Method : other: Application of the chicken embryo in testing for embryotoxicity, Korhonen et al., 1982

Year :
GLP : no data
Test substance : no data

Method : Three day (72-76 hr) chicken embryos were selected by candling. The test compound, in 5 ul acetone, was injected into the heart of the embryo. Two days after injection, the eggs were candled again. Eggs containing dead embryos were counted and discarded. The remaining eggs were candled every second or third day. Those containing dead embryos were opened, and the embryos examined for external malformations and for the stage of development. Incubation was terminated after 11 days (total incubation

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time of 14 days), and the remaining eggs were opened and inspected for survival and external malformations. Embryos were classified according to time of death, stage of development and type of malformations. LD50 and ED50 values were calculated according to the method of Rosiello, et al. (1977).

Result : The test compound, even the highest doses (1.0 umoles/egg), did not induce any effects (early death, defects or malformations) above those of the background (vehicle) acetone.

Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment - avian rather than mammalian study.

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(39) (40)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6. Analyt. Meth. for Detection and Identification

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6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

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7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8. Meas. Nec. to Prot. Man, Animals, Environment

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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

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9. References

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10. Summary and Evaluation

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Date 18.06.2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical : ID: 2492-26-4
CAS No. : 2492-26-4
EINECS Name : sodium benzothiazol-2-yl sulphide
EC No. : 219-660-8
TSCA Name : 2(3H)-Benzothiazolethione, sodium salt
Molecular Formula : C7H5NS2.Na

Producer related part
Company : Bayer Corporation
Creation date : 13.10.1999

Substance related part
Company : Bayer Corporation
Creation date : 13.10.1999

Status :
Memo : American Chemistry Council, Rubber and Plastic Additives Panel,
Benzothiazole-based Thiazoles Category

Printing date : 18.06.2003
Revision date :
Date of last update : 18.06.2003

Number of pages : 42

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. General Information

Id 2492-26-4

Date 18.06.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation
Name : American Chemistry Council, Rubber and Plastic Additives Panel (RAPA)
Contact person :
Date :
Street : 1300 Wilson Boulevard
Town : 22209 Arlington, VA
Country : United States
Phone : 703-741-5600
Telefax : 703-741-6091

18.06.2003

Type : cooperating company
Name : Bayer Polymers LLC (a wholly -owned subsidiary of Bayer Corporation)
Contact person :
Date :
Street : 100 Bayer Road
Town : 15205-9741 Pittsburgh, PA
Country : United States

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Type : cooperating company
Name : Crompton Corporation
Contact person :
Date :
Street : Benson Road
Town : 06749 Middlebury, CT
Country : United States

18.06.2003

Type : cooperating company
Name : Flexsys America L.P.
Contact person :
Date :
Street : 260 Springdale Drive
Town : 44333-0444 Akron, OH
Country : United States

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Type : cooperating company
Name : Noveon, Inc.
Contact person :
Date :
Street : 9911 Brecksville Road
Town : 44141-3247 Cleveland, OH
Country : United States

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1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1. General Information

Id 2492-26-4
Date 18.06.2003

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name : 2(3H)-benzothiazolethione, sodium salt
Smiles Code : [Na]c12nc(S)sc1cccc2
Molecular formula : C7H5NS2.Na
Molecular weight : 189.23
Petrol class :

15.04.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : liquid
Purity : > 95 % w/w
Colour : Yellow to brown oily liquid
Odour :

Remark : This substance is only supplied as aqueous solutions (18-50%).

18.06.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2(3H)-benzothiazolethione sodium salt

20.10.1999

2-mercaptobenzothiazole, sodium salt

15.04.2003

NACAP®

15.04.2003

NaMBT

15.04.2003

SMBT

20.10.1999

Sodium 2-Mercaptobenzothiazole

15.04.2003

Sodium benzothiazol-2-yl sulphide

15.04.2003

Sodium MBT

20.10.1999

1. General Information

Id 2492-26-4
Date 18.06.2003

Sodium Mercaptobenzothiazole

15.04.2003

1.3 IMPURITIES

Purity :
CAS-No : 1310-73-2
EC-No :
EINECS-Name : Sodium hydroxide (Na(OH))
Molecular formula :
Value : < .5 % v/v

15.04.2003

Purity :
CAS-No : 7757-82-6
EC-No :
EINECS-Name : Sulfuric acid disodium salt
Molecular formula :
Value : < .5 % v/v

15.04.2003

Purity :
CAS-No : 7647-14-5
EC-No :
EINECS-Name : Sodium chloride (NaCl)
Molecular formula :
Value : < .4 % v/v

15.04.2003

1.4 ADDITIVES

Purity type :
CAS-No : 7732-18-5
EC-No : 231-791-2
EINECS-Name : water
Molecular formula :
Value : 50 - 82 % v/v
Function of additive :

15.04.2003

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1. General Information

Id 2492-26-4
Date 18.06.2003

1.7 USE PATTERN

Type of use : type
Category : Non dispersive use

20.10.1999

Type of use : type
Category : Use resulting in inclusion into or onto matrix

20.10.1999

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

20.10.1999

Type of use : industrial
Category : Polymers industry

20.10.1999

Type of use : use
Category : Corrosive inhibitors

20.10.1999

Type of use : use
Category : Intermediates

20.10.1999

Type of use : use
Category : Vulcanizing agents

20.10.1999

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

Type : TSCA
Additional information :

15.04.2003

2. Physico-Chemical Data

Id 2492-26-4

Date 18.06.2003

2.1 MELTING POINT

Value	:	= -6 °C	
Decomposition	:	no, at °C	
Sublimation	:	no	
Method	:	other: FF88.2-1, Crystallizing Point of Organic Compounds, 1997	
Year	:		
GLP	:	yes	
Test substance	:	other TS: 50% solution NaMBT	
Remark	:	Freezing point/crystallizing point for 50% aqueous solution	
Reliability	:	(1) valid without restriction GLP guideline study	
Flag	:	Critical study for SIDS endpoint	(1)
15.04.2003			
Value	:	159.8 - 180.4 °C	
Remark	:	Melting point for pure Sodium MBT, a highly hydroscopic solid GLP study	
15.04.2003			(2)

2.2 BOILING POINT

Value	:	= 103 °C at 1013 hPa	
Decomposition	:	no	
Method	:	other: no data	
Year	:		
GLP	:	no data	
Test substance	:	other TS: 50% solution NaMBT	
Remark	:	Boiling point is for a 50% aqueous solution of sodium 2-mercaptobenzothiazole.	
Reliability	:	(2) valid with restrictions no method detail	
Flag	:	Critical study for SIDS endpoint	(3)
15.04.2003			

2.3 DENSITY

Type	:	relative density	
Value	:	= 1.25 at 25 °C	
Method	:		
Year	:		
GLP	:	no data	
Test substance	:		
Flag	:	Critical study for SIDS endpoint	(4)
16.04.2003			
Type	:	density	
Value	:	ca. 1.3 g/cm ³ at 25 °C	
Method	:	other: FF97.4/ASTM D891-94, 1997	
Year	:		
GLP	:	yes	
Test substance	:		

2. Physico-Chemical Data

Id 2492-26-4

Date 18.06.2003

Remark : Specific Gravity of Liquids by Hydrometers. Hydrometers must meet ASTM E100 specifications.
15.04.2003 (5)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : 34.2639 hPa at 30 °C
Decomposition :
Method : other (measured)
Year :
GLP : no data
Test substance : other TS: 47-50% aqueous solution NaMBT

Remark : The vapour pressure of pure NaMBT is expected to be extremely low. The values listed reflects the water content of a 47-50% aqueous solution rather than that of the pure compound.

Result : Vapor Pressure =
59.9951 hPa @ 40°C
173.319 hPa @ 60°C
283.310 hPa @ 70°C
433.298 hPa @ 80°C

Reliability : (2) valid with restrictions
no method detail

Flag : Critical study for SIDS endpoint
15.04.2003 (6)

Value : = 32 hPa at 25 °C
Decomposition :
Method : other (measured): no data
Year :
GLP : no data
Test substance :

Remark : Vapour pressure of sodium 2-mercaptobenzothiazole would be expected to extremely low. The vapor pressure listed is due to the water present in the aqueous solution and not due to sodium 2-mercaptobenzothiazole.

Source : Monsanto Europe N.V. Bruxelles
15.04.2003 (7)

Value : 34.2639 hPa at 25 °C
Decomposition :
Method : other (measured)
Year :
GLP : no data
Test substance :

Remark : Data from US EPA R.E.D., Sodium and Zinc Salts of 2-MBT.
15.04.2003 (2) (8)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : = -.46 at 25 °C
pH value :
Method : other (measured): HPLC Method for Pow, 1978
Year : 1978

2. Physico-Chemical Data

Id 2492-26-4

Date 18.06.2003

GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : 1% and .01% solutions in 100 ml n-Octanol added to 500 ml water.
Shaken for 48 hours, equilibration for several days.
Equilibration performed in the dark to preclude photodegradation. Analysis via HPLC to determine Pow.
Pow = 0.34 +/- 0.18

Reliability : (2) valid with restrictions
no method detail

Flag : Critical study for SIDS endpoint
16.04.2003 (9)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in Value : Water
: at °C
pH value concentration : 11.5 - 13.5
: 100 vol% at 25 °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : miscible
Stable :
Deg. product :
Method : other: Saturated Solution / HPLC Analysis, 1978
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : 25 ml of the test substance and 500 ml purified water was stirred for several days in the dark. After filtration and centrifugation, the solution was analyzed via HPLC (50:50 acetonitrile and water, 325 mn).
pH Method: FF83.11-1, pH Values of Aqueous Solutions, Suspensions and Emulsions by Potentiometry, 1997.
- measured using a pH meter with an accuracy of +/- 0.1 pH.

Reliability : (2) valid with restrictions
no method detail

Flag : Critical study for SIDS endpoint
15.04.2003 (9)

Solubility in Value : Water
: > 500 g/l at 25 °C
pH value concentration : = 11.5 - 13.5
: 50 vol% at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other
Year :
GLP : no data
Test substance :

Source : Monsanto Europe N.V. Bruxelles
15.04.2003 (10)

Solubility in : Water

2. Physico-Chemical Data

Id 2492-26-4

Date 18.06.2003

Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : 11.6 at 25 °C
Description :
Stable :

15.04.2003

(2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : > 104.4 °C
Type : closed cup
Method : other: ASTM D 56-96, 1996
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (1) valid without restriction
Guideline study

15.04.2003

(11)

Value : > 93 °C
Type : other
Method :
Year :
GLP : no data
Test substance :

Source : Monsanto Europe N.V. Bruxelles

15.04.2003

(10)

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

Memo : Henry's Law Constant

Method : calculated: EPIWIN/HENRYWIN v3.10
Remark : Calculated at 25°C using measured values for water solubility, Vapor pressure and Log Kow.

Result : 0.0064 atm·m³/mole

Reliability : (2) valid with restrictions
Accepted calculation method

15.04.2003

(12)

3. Environmental Fate and Pathways

Id 2492-26-4

Date 18.06.2003

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 : .00000000045129 cm³/(molecule*sec)
Degradation : 50 % after 2.8 hour(s)
Deg. product :
Method : other (calculated): AopWin v1.89
Year : 2000
GLP : no
Test substance : other TS: molecular structure

Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
15.04.2003

(12)

3.1.2 STABILITY IN WATER

Type : abiotic

Result : Below pH 7, NaMBT will be protonated to form insoluble MBT.
If iron is present, NaMBT will be reduced to benzothiazole.
In aqueous solution, NaMBT is not oxidized, even at temperatures of 100°C, nor is it readily hydrolyzed.
In weak alkaline or neutral solutions, the mercaptobenzothiazole (MBT) anion can readily complex with various metal ions and form insoluble, relatively undissociable salts.

Reliability : (4) not assignable
Secondary literature

15.04.2003

(13)

Type : abiotic
Degradation : 15 % after 7 day(s) at pH 7 and °C
Deg. product :
Method : other: Monsanto protocol
Year : 1985
GLP : yes
Test substance : other TS: 2-mercaptobenzothiazole, purity = 98%

Remark : Sodium MBT will dissociate to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thiazoles category of chemicals.

Reliability : (1) valid without restriction
GLP study

18.06.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3. Environmental Fate and Pathways

Id 2492-26-4

Date 18.06.2003

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air, water, soil, sediment
Method : other: Level III Fugacity Model, EPISUITE/EPIWIN v3.10
Year : 2000

Remark : Calculation based on molecular structure and measured water solubility, vapour pressure and Log Kow.
Modeling was performed using equal releases (1000 kg/hr) and equal distribution to all compartments.

Result :

	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	8.31	5.69	1000	7.72e-012
Water	85.6	360	1000	4.06e-013
Soil	5.95	360	1000	2.76e-012
Sediment	0.143	1.44e+003	0	2.71e-013

Persistence Time: 73.7 hr

Reliability : (2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint
16.04.2003 (12)

Type : volatility
Media : water - air
Method : other: Estimation Method, 1990
Year :

Remark : Model river = 1 m deep flowing at 1 m/sec and wind velocity of 3 m/sec.
Model lake = 1 m deep flowing at 0.05 m/sec and wind velocity of 0.5 m/sec.

Result : Volatilization half-life from model river: 1.53 hours
Volatilization half-life from model lake: 132 hours
Volatilization Constant from water: 0.0064 atm·m³/mole

Reliability : (2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint
16.04.2003 (14)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 23.8 mg/l related to Test substance related to

Contact time :
Degradation : < 1 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Deg. product :
Method : EPA OTS 796.3100
Year : 1989
GLP : yes
Test substance : **other TS: 2-mercaptobenzothiazole, purity = 98%**

Method : Gledhill method listed in U.S. TSCA regulations 40 CFR Ch 1 subpart D paragraph 796.3100

Remark : Sodium MBT will dissociate to 2-MBT, this study on 2-MBT is used to fill

3. Environmental Fate and Pathways

Id 2492-26-4

Date 18.06.2003

Reliability : this endpoint in the Benzothiazole-based thioles category of chemicals.
: (1) valid without restriction
GLP guideline study
18.06.2003

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species : other
Exposure period : at °C
Concentration :
BCF : 1
Elimination :
Method : other: Calculation, Neely, et. al., 1974
Year :
GLP : no
Test substance : other TS: Calculation from measured octanol/water partition coefficient of NaMBT

Result : BCF= 1 (+/- 1)
Calculation from measured octanol/water partition coefficient $Pow = 0.34$
(+/- 0.18)

Reliability : (2) valid with restrictions
Accepted calculation method
16.04.2003 (9)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 2492-26-4

Date 18.06.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	: static
Species	: Lepomis macrochirus (Fish, fresh water)
Exposure period	: 96 hour(s)
Unit	: mg/l
NOEC	: 2.1
LC50	: = 3.8
LOEC	: 2.8
Limit test	:
Analytical monitoring	: no
Method	: other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians
Year	: 1975
GLP	: no data
Test substance	: as prescribed by 1.1 - 1.4
Result	: LC50 (24h) = 5.7 mg/l LC50 (48h) = 4.5 mg/l LC50 (96h) = 3.8 mg/l Conf.Int.=3.2-4.4 mg/l NOEC = 2.1 mg/l LOEC = 2.8 mg/l
Test condition	: The test material, in reagent-grade acetone, was introduced into 15 liters of diluent water in all-glass vessels. Nominal test concentrations (duplicate) were 0, 2.1, 2.8, 3.2, 3.7, 4.9, 6.5 or 10 mg/l, plus a solvent (acetone) control. To each test vessel, 10 bluegill, standard length 3.8 cm, were then added. The test fish were not fed 48 hours prior to testing, nor during exposure. No aeration was provided during the test, and temperature was maintained at 22°C. Dissolved oxygen ranged from 8.8 mg/l (100% saturation) to 0.3 mg/l (3% saturation) from beginning to end of exposure, respectively. pH values ranged from 7.2 initially, to 6.7 at the end of the test. Observations and mortality counts were made every 24 hours. Test concentrations and observed percentage mortality were converted to logarithms and probits, respectively, and these values were utilized in a least squares regression analysis. The LC50s and the 95% confidence intervals were calculated from the regression equation.
Reliability	: (2) valid with restrictions age of study, lack of method detail
Flag	: Critical study for SIDS endpoint
14.05.2003	(15)
Type	: static
Species	: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	: 96 hour(s)
Unit	: mg/l
NOEC	: 1.4
LC50	: 1.8
LOEC	: 1.8
Limit test	:
Analytical monitoring	: no
Method	: other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians
Year	: 1975
GLP	: no data
Test substance	: as prescribed by 1.1 - 1.4
Result	: LC50 (24h) = 2.0 mg/l LC50 (48h) = 1.8 mg/l LC50 (96h) = 1.8 mg/l NOEC = 1.4 mg/l

4. Ecotoxicity

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Test condition : LOEC = 1.8 mg/l
: The test material, in reagent-grade acetone, was introduced into 15 liters of diluent water in all-glass vessels. Nominal test concentrations (duplicate) were 0, 1.0, 1.4, 1.8, 2.4, or 3.2 mg/l, plus a solvent (acetone) control. To each test vessel, 10 rainbow trout, standard length 3.7 cm, were then added. The test fish were not fed 48 hours prior to testing, nor during exposure. No aeration was provided during the test, and temperature was maintained at 12°C. Dissolved oxygen ranged from 9.5 mg/l (89% saturation) to 2.4 mg/l (22% saturation) from beginning to end of exposure, respectively. pH values ranged from 7.3 initially, to 6.7 at the end of the test. Observations and mortality counts were made every 24 hours. Test concentrations and observed percentage mortality were converted to logarithms and probits, respectively, and these values were utilized in a least squares regression analysis. The LC50s and the 95% confidence intervals were calculated from the regression equation.

Reliability : (2) valid with restrictions
age of study, lack of method detail

Flag : Critical study for SIDS endpoint

14.05.2003

(16)

Type : static

Species : Lepomis macrochirus (Fish, fresh water)

Exposure period : 96 hour(s)

Unit : mg/l

LC50 : 12 - 15

Limit test :

Analytical monitoring : no data

Method : other: according to Northeastern Biologists (1976)

Year :

GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Remark : The toxic effect took place during the first 24 hours of exposure.

Result :

Concentration (mg/l)	% mortality				
	24hrs	48hrs	72hrs	96hrs	Total
9.5	0	0	0	0	0
12.00	5	0	0	0	5
15.00	95	0	0	0	95
Control	0	0	0	5	5

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

14.05.2003

(17)

Type : static

Species : Oncorhynchus mykiss (Fish, fresh water)

Exposure period : 96 hour(s)

Unit : mg/l

NOEC : 1.99

LC50 : 2.58 - 3.16

LOEC : 2.58

Method : other: according to Northeastern Biologists (1976)

Year :

GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Remark : The toxic effect took place during the first 24 hours of exposure.

4. Ecotoxicity

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Date 18.06.2003

Result : Concentration % mortality
(mg/l) 24hrs 48hrs 72hrs 96hrs Total
1.99 0 0 0 0 0
2.58 15 0 0 0 15
3.16 75 0 0 0 75
Control 0 0 0 0 0

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

14.05.2003

(17)

Type : static
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 1.8
Limit test :
Analytical monitoring : no
Method : other: Bionomics Laboratory protocol; see test conditions
Year : 1976
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : C.I.=1.3-2.4 mg/l; 24hr LC50=2.0 mg/l; 48hr LC50=1.8 mg/l
Source : Monsanto Europe N.V. Bruxelles
Test condition : carrier-acetone; 15 L dilution water; length=3.7 cm; no food; temp=12C

24.05.1994

(18)

Type : static
Species : Oncorhynchus tshawytscha (Fish, fresh water, marine)
Exposure period : 4 hour(s)
Unit : mg/l
LC100 : 10
Limit test :
Analytical monitoring : no
Method : other: MacPhee, C. et al protocol; see test conditions
Year : 1969
GLP : no data
Test substance : no data

Remark : fish died after 2-4 hour exposure at 10 mg/l
Source : Monsanto Europe N.V. Bruxelles
Test condition : fish 5-10 cm long; acclimated; river water; temp=11C

26.04.2001

(19)

Type : static
Species : Ptychocheilus oregonensis (Fish, fresh water)
Exposure period : 11 hour(s)
Unit : mg/l
LC100 : 10
Limit test :
Analytical monitoring : no data
Method : other: MacPhee, C. et al protocol; see test conditions
Year : 1969
GLP : no data
Test substance : no data

Remark : fish died after 7-11 hour exposure at 10 mg/l
Source : Monsanto Europe N.V. Bruxelles
Test condition : fish 5-10 cm long; acclimated; river water; temp=11C

26.04.2001

(19)

4. Ecotoxicity

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Date 18.06.2003

Type :
Species : Leuciscus idus (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : > 5
Limit test :
Analytical monitoring : no data
Method : other: test conditions undocumented
Year : 1985
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
26.05.1994 (20)

Type :
Species : Poecilia reticulata (Fish, fresh water)
Exposure period : 48 hour(s)
Unit :
Method : other
Year :
GLP :
Test substance : other TS: UniRoyal NaMBT; purity not noted

Result : TLm = 12 ppm (48 hours) in tap water
26.04.2001 (21)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : = 10
EC50 : = 19
Analytical monitoring : no
Method : other: Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA Ecological Research Series EPA-660/3-75-009 April 1975
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Test condition : The Daphnia magna used in the test were cultured at the ABC facilities. Adult Daphnia were fed the algae Selenastrum capricornutum at least every three days prior to testing and supplemented with a suspension of trout chow. The bioassay was conducted in 250ml glass beakers containing 200 ml of ABC well water. Dissolved oxygen concentration was 8.6 ppm, pH was 7.7, alkalinity was 210 mg/l and hardness (CaCO₃) was 220 ppm. Vessels were kept at 20°C in a temperature-controlled area. Lighting was maintained at 50-70 foot-candles on a 16-hour daylight photoperiod. An initial range-finding experiment was carried out to determine the exposure concentrations for the definitive test. Acetone was used as the solvent for the test solutions, and the experiment included both a control and a solvent control. The compound was tested over a range from 10 to 56 mg/l. Ten Daphnia, first instar less than 24 hours old, were selected for each (duplicate) test concentration. Daphnia in all concentrations were observed once every 24 hours for mortality and abnormal effects. Dissolved oxygen level was >7.0 ppm and pH was 8.1 at the termination of the test. These values were considered adequate and equivalent to those measurements

4. Ecotoxicity

Id 2492-26-4

Date 18.06.2003

in the control chamber. The LC50 values and 95% confidence intervals were calculated employing the statistical technique of Litchfield and Wilcoxon (1949).

Reliability : (1) valid without restriction
GLP guideline study

Flag : Critical study for SIDS endpoint

14.05.2003 (22)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : growth rate
Exposure period : 96 hour(s)
Unit :
Limit test :
Analytical monitoring : no
Method : other: Selastrum capricornutum Algal Assay Bottle Test (1971), closed system
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Result : EC50 (24h) = 2 ppm
EC50 (96h) = 0.4 ppm (biomass)
EC50 (96h) = 0.3 ppm (growth rate)
NOEC = Not determined
LOEC = 0.3 ppm

Test condition : The test algae were obtained from the US EPA Environmental Research Laboratory in Corvallis, Oregon. Beginning cell numbers in the test flasks were 1.0×10^4 cells/ml. Cultures were incubated at 24°C under approximately 4,300 lux illumination. Triplicate cultures were employed for each of the test concentrations and the control. Test containers were 125ml flasks containing 50ml of test medium. Concentrations for the definitive test were based on the results of a 72-hr range-finding study. These concentrations were 0, 0.3, 0.6, 1, 3 or 6 ppm. Water was used to prepare the stock solutions and as the solvent control. The pH values ranged from 7.8 at the beginning of the study, to 7.1 at the 96-hour mark for the test compound and 8.2 for the water control. There were no other water quality measurements reported in this study. Statistical analysis involved converting each test concentration to a logarithm, and the corresponding percentage decrease of in vivo chlorophyll a or cell numbers was converted to a probit (Finny, 1971). The EC50s and 95% confidence limits were then calculated by linear regression.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

18.06.2003 (23)

Species : Selenastrum capricornutum (Algae)
Endpoint : biomass
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : .3
Limit test :
Analytical monitoring : no
Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year : 1984
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

4. Ecotoxicity

Id 2492-26-4

Date 18.06.2003

Result : C.I.=.04-3 mg/l;
in vivo chlorophyll EC50:
24hr= 2 mg/l;
48hr= 1 mg/l;
72hr= 0.4 mg/l;
96hr= 0.4 mg/l

Source : Monsanto Europe N.V. Bruxelles

Test condition : temp=24C; 4000 lux

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint

18.06.2003

(24)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type :
Species : activated sludge

Exposure period : 3 hour(s)

Unit : mg/l

EC50 : = 857

Analytical monitoring : no data

Method : ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"

Year :
GLP : yes

Test substance : no data

Remark : Direct weighing in, nominal concentration, high bacteria density

Source : Monsanto Europe N.V. Bruxelles

Reliability : (1) valid without restriction
GLP guideline study

16.04.2003

(25)

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. Toxicity

Id 2492-26-4

Date 18.06.2003

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : 1476 mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals :
Vehicle :
Doses :
Method : EPA OPP 81-1
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Result : LD50: 1476 mg/kg bw (combined sexes)
LD50: 1615 mg/kg bw (males)
LD50: 1337 mg/kg bw (females)

Reliability : (1) valid without restriction
GLP guideline study

Flag : Critical study for SIDS endpoint

16.04.2003

(26)

Type : LD50
Value : = 4350 mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 20
Vehicle : other: none, undiluted
Doses : 2510, 3160, 3980 or 5010 mg/kg bw
Method : other: Younger Laboratory Single Oral Dose Protocol, 1974
Year : 1974
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : The test material was administered to four groups of male and female rats (5 animals/dose level) undiluted. Dose levels were 2510, 3160, 3980 or 5010 mg/kg body weight. Male rats had initial body weights ranging from 215-245 grams: females had initial body weights ranging from 200-235 grams.

Result : Clinical signs of intoxication were reduced appetite and activity (lasting up to one day in survivors), rapidly increasing weakness, tremors, convulsions, collapse and death. Deaths occurred one hour to one day after dosing, with most within two hours of dosing. After a 14-day observation period, survivors were sacrificed. Gross autopsy findings on decedents were hemorrhagic areas of the lungs, liver hyperemia and acute gastrointestinal inflammation. There were no findings in survivors; all viscera appeared normal.

Dose mg/kg	Mortalities		
	Male	Female	Combined
2510	0/3	0/2	0/5
3160	0/2	2/3	2/5
3980	1/3	1/2	2/5
5010	1/2	3/3	4/5

Reliability : (2) valid with restrictions
age of study, lack of method detail

Flag : Critical study for SIDS endpoint

16.04.2003

(27)

5. Toxicity

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Type : LD50
Value : = 5200 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Younger Laboratory method
Year : 1978
GLP : no data
Test substance : other TS

Source : Monsanto Europe N.V. Bruxelles
Test substance : 45% to 50% substance content.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
20.10.1999

(28)

Type : LD50
Value : = 9500 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Younger Laboratory method
Year : 1987
GLP : yes
Test substance : other TS

Source : Monsanto Europe N.V. Bruxelles
Test substance : 22% substance content.
01.06.1994

(29)

Type : LD50
Value : = 2160 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1973
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
23.05.1994

(30)

Type : LD50
Value : = 3968 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity

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Date 18.06.2003

Year : 1975
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
23.05.1994

(31)

Type : LD50
Value : = 750 mg/kg bw
Species : rat
Strain :
Sex : male
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1965
GLP : no data
Test substance : other TS

Result : Dose mortality
(ml/kg)
0.625 1/5
1.25 2/5
2.5 3/5
5.0 5/5

Signs of intoxication: tremors, convulsion, severe depression and hematuria.

Gross autopsy findings: decedents - hemorrhage of stomach
survivors - normal

Source : Monsanto Europe N.V. Bruxelles
Test substance : 50% Na-2-mercaptobenzothiazole solution
14.05.2003

(32)

Type : LD50
Value : = 3120 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1980
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
23.05.1994

(33)

Type : LD100
Value : = 2500 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1975

5. Toxicity

Id 2492-26-4

Date 18.06.2003

GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
23.05.1994 (34)

Type : LD100
Value : = 3125 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1965
GLP : no data
Test substance : other TS

Remark : male rats only
Source : Monsanto Europe N.V. Bruxelles
Test substance : 50% Na-2-mercaptobenzothiazole
03.06.1994 (32)

Type : other
Value : > 625 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1975
GLP : no data
Test substance : no data

Remark : male rat mortality:
1) 312.5 mg/kg bw - 1/5
2) 625 mg/kg bw - 2/5
3) 1250 mg/kg bw - 3/5
Source : Monsanto Europe N.V. Bruxelles
23.05.1994 (35)

Type : other
Value : > 391 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1965
GLP : no data
Test substance : other TS

Remark : male rat mortality:
1) 391 mg/kg bw, 1/5
2) 782 mg/kg bw, 2/5
3) 1563 mg/kg bw, 3/5

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Id 2492-26-4

Date 18.06.2003

Source : Monsanto Europe N.V. Bruxelles
Test substance : 50% Na-2-mercaptobenzothiazole
03.06.1994 (32)

Type : other
Value : 2000 - 3980 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1963
GLP : no data
Test substance : no data

Remark : Dose: mortality:
2000 mg/kg bw 0/2
3980 mg/kg bw 3/3

Source : Monsanto Europe N.V. Bruxelles
16.05.2003 (36)

Type : LD50
Value : = 1792 mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1948
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
23.05.1994 (37)

Type : LD0
Value : = 708 mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Acute Oral Toxicity
Year : 1948
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
23.05.1994 (38)

Type : LD100
Value : = 2560 mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :

5. Toxicity

Id 2492-26-4

Date 18.06.2003

Doses :
Method : other: Acute Oral Toxicity
Year : 1948
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
23.05.1994

(37)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Value : > 1.3 mg/l
Species : rat
Strain : Sprague-Dawley
Sex : male
Number of animals : 6
Vehicle : other: None - undiluted
Doses : 1.3 mg/l
Exposure time : 6 hour(s)
Method : other: A.T.S., 1973
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : There were no signs of toxicity noted, and all rats survived. After an uneventful 14-day observation period, the test animals were sacrificed. All viscera appeared normal in these animals.

Test condition : Six male rats were exposed to the test substance in a stream of ambient (27°C) air for six hours. Chamber humidity was 85%, chamber volume was 35 liters, and the air flow rate was 4.0 liters/minute. The difference in weights between the initial sample and the recovered sample was 1.9 grams, for a calculated concentration of 1.3 mg/l.

Reliability : (2) valid with restrictions
age of study, lack of method detail

Flag : Critical study for SIDS endpoint
16.04.2003

(39)

Type : LC50
Value : > 6.5 mg/l
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Exposure time : 6 hour(s)
Method : other: Younger Laboratory method
Year : 1978
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Monsanto Europe N.V. Bruxelles
16.04.2003

(40)

Type : LC50
Value : > 8.2 mg/l
Species : rat
Strain :
Sex :

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Id 2492-26-4

Date 18.06.2003

Number of animals :
Vehicle :
Doses :
Exposure time : 6 hour(s)
Method : other: Younger Laboratory method
Year : 1987
GLP : yes
Test substance : other TS

Source : Monsanto Europe N.V. Bruxelles
Test substance : 22% substance content.
Reliability : (1) valid without restriction
20.10.1999

(29)

Type : LC50
Value :
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Exposure time : 7 hour(s)
Method : other: Acute Inhalation Toxicity
Year : 1963
GLP : no data
Test substance : no data

Remark : Exposure to a saturated atmosphere resulted in 0/4 mortality
Source : Monsanto Europe N.V. Bruxelles
23.05.1994

(41)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > 7940 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 3
Vehicle : other: None - undiluted
Doses : 5010 or 7940 mg/kg bw
Method : other: Younger Laboratory Single Dermal Dose Protocol, 1974
Year : 1974
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Clinical signs of toxicity included slightly reduced appetite and activity for four to seven days. There were no mortalities at any dose level. All animals survived until sacrifice on Day 14. Gross autopsy reports indicated that all viscera appeared normal.

Dose mg/kg	Mortalities		
	Male	Female	Combined
5010	0/1	----	0/1
7940	0/1	0/1	0/2

Test condition : The test substance, undiluted, was applied to the shaved skin of two groups of male and female rabbits for 24 hours as single dermal application at dose levels of 5010 or 7940 mg/kg/body weight. Body weights of males

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were 2.3 and 2.6 kg, and the female weighed 2.4 kg. The test material was held in place by means of an occlusive wrap of latex rubber and secured by bandaging and elastic tape. The occlusive wrap was removed after 24 hours and the excess material was wiped from the test animal. Clinical observations were made three times during the first eight hours after dosing, and twice daily thereafter until sacrifice.

Reliability : (2) valid with restrictions
age of study, lack of method detail
Flag : Critical study for SIDS endpoint
16.04.2003 (42)

Type : LD50
Value : > 5010 mg/kg bw
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Younger Laboratory method
Year : 1978
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Monsanto Europe N.V. Bruxelles
Test substance : 45% to 50% substance content.
03.06.1994 (28)

Type : LD50
Value : > 7940 mg/kg bw
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: Younger Laboratory method
Year : 1987
GLP : yes
Test substance : other TS

Source : Monsanto Europe N.V. Bruxelles
Test substance : 22% substance content.
Reliability : (1) valid without restriction
20.10.1999 (29)

Type : LD50
Value : > 1250 mg/kg bw
Species : rabbit
Strain :
Sex :
Number of animals : 10
Vehicle :
Doses : 1.25, 2.5, 5.0 ml/kg (313, 625, 1250 mg/kg bw)
Method : other: Acute Dermal Toxicity
Year : 1975
GLP : no data
Test substance : other TS

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Remark	:	Dose	mortality
		(ml/kg) (mg/kg bw)	
		1.25 313	0/10
		2.5 625	1/10
		5.0 1250	4/10
		Signs of intoxication: severe depression, cold extremities, appetite loss.	
		Skin irritation: severe degree of skin injury. Area burned at 24 hours with formation of hard eschar at 1-2 weeks.	
Source	:	Monsanto Europe N.V. Bruxelles	
Test substance	:	50% Na-2-mercaptobenzothiazole	
16.05.2003			(43)
Type	:	LD50	
Value	:	> 3125 mg/kg bw	
Species	:	rabbit	
Strain	:		
Sex	:	male	
Number of animals	:	10	
Vehicle	:		
Doses	:	782, 1563, 3125 mg/kg bw	
Method	:	other: Acute Dermal Toxicity	
Year	:	1965	
GLP	:	no data	
Test substance	:	other TS	
Remark	:	<u>Dose:</u>	<u>mortality:</u>
		782 mg/kg bw,	0/10
		1563 mg/kg bw,	1/10
		3125 mg/kg bw,	4/10
Source	:	Monsanto Europe N.V. Bruxelles	
Test substance	:	50% Na-2-mercaptobenzothiazole	
16.05.2003			(44)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Exposure	:	Semiocclusive
Exposure time	:	24 hour(s)
Number of animals	:	6
Vehicle	:	other: none
PDII	:	8
Result	:	corrosive
Classification	:	corrosive (causes burns)
Method	:	other: Younger Laboratories Protocol D.1.30, 1984
Year	:	1987
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	The results indicated that application of the test article induced cratering and injury in depth, and the material should be classified as corrosive.
Test condition	:	The undiluted test article, at a volume of 0.5 ml, was applied to two sites on the shaved intact skin of six rabbits for 4 hours and held in place with a semi-occlusive dressing. The initial observation was made approximately

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one hour after exposure. Dermal irritation was scored by the Draize Method, and results recorded at 24, 48, 72 and 168 hours after exposure. Each patch position was scored for erythema and edema.

Reliability	:	(1) valid without restriction GLP study	
16.04.2003			(45)
Species	:	rabbit	
Concentration	:	undiluted	
Exposure	:	Semioclusive	
Exposure time	:	24 hour(s)	
Number of animals	:	6	
Vehicle	:		
PDII	:	6.6	
Result	:	highly irritating	
Classification	:	irritating	
Method	:	other: Draize et al., 1944	
Year	:	1974	
GLP	:	no data	
Test substance	:	as prescribed by 1.1 - 1.4	
Method	:	Draize, J.H. Woodard, G., and Calvery, H.O., Methods for the Study of Irritation and Toxicity of Substances Applied Topically To the Skin and Mucous Membranes, J. Pharmacol. Exp. Therap. 82: 377-390, 1944	
Result	:	At 24 hours, necrosis and severe edema were noted. Application of the test compound had a severe defatting effect. Skin sloughed off in ten to fourteen days. However, there was no injury in depth. Primary skin irritation score was 6.6/8.0	
Test condition	:	The undiluted test article, at a volume of 0.5 ml, was applied to the intact and abraded shaved skin of six rabbits for 24 hours. The initial observation was made approximately one hour after exposure. Dermal irritation was scored by the Draize Method, and results recorded on day 1, 3, 7, 10, 14 and 17 after exposure.	
Reliability	:	(2) valid with restrictions age of study, lack of method detail	
16.04.2003			(46)
Species	:	rabbit	
Concentration	:		
Exposure	:		
Exposure time	:		
Number of animals	:		
Vehicle	:		
PDII	:		
Result	:	corrosive	
Classification	:		
Method	:	other: Younger Laboratory method	
Year	:	1978	
GLP	:	no data	
Test substance	:	other TS	
Remark	:	Use of 24-hour exposure data prohibits direct classification.	
Source	:	Monsanto Europe N.V. Bruxelles	
Test substance	:	45% to 50% substance content.	
03.06.1994			(28)
Species	:	rabbit	
Concentration	:		
Exposure	:		
Exposure time	:		
Number of animals	:		

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Vehicle :
PDII :
Result : corrosive
Classification : corrosive (causes burns)
Method : other: Younger Laboratory method
Year : 1978
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Monsanto Europe N.V. Bruxelles
Test substance : 45% to 50% substance content.
03.06.1994

(47)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : highly corrosive
Classification :
Method : other: Skin Irritation
Year : 1975
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
27.05.1994

(35)

Species : human
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : slightly irritating
Classification :
Method : other: Skin Irritation
Year : 1962
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
27.05.1994

(48)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : .1 ml
Exposure time :
Comment : not rinsed
Number of animals : 6
Vehicle : none
Result : moderately irritating
Classification : irritating
Method : other: Draize, J.H., Woodard, G., and Calvery, H.O., 1944
Year : 1974

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GLP	:	no data	
Test substance	:	as prescribed by 1.1 - 1.4	
Result	:	Immediate: severe discomfort, pawing, thrashing, closed eyes 10 min: Severe erythema, moderate edema, copious discharge 1 hour: Barely perceptible/slight areas of corneal cloudiness, sluggish iris reaction to light, necrosis in conjunctival sac, moderate edema, copious discharge 24 hours: barely perceptible/slight areas of corneal cloudiness, sluggish iris reaction to light, necrosis in conjunctival sac, moderate edema, copious discharge containing white exudate 48 -120 hours: Gradual improvement 168 hours: All animals scored "0" The average Draize score for 24, 48 and 72 hours was calculated for each animal and then averaged over the six animals. The average Draize score was 22.5 on a scale from 0-110.	
Test condition	:	0.1 ml of the undiluted test substance was applied to one eye of six albino rabbits. The other eye was not treated and served as a control. The cornea, iris and conjunctiva were examined immediately after treatment, and then at intervals of 1 hour, 10 minutes, and at 24, 48, 72 and 168 hours. The Draize Method was used for scoring eye irritation.	
Reliability	:	(2) valid with restrictions age of study, lack of method detail	
16.04.2003			(49)
Species	:	rabbit	
Concentration	:		
Dose	:		
Exposure time	:		
Comment	:		
Number of animals	:		
Vehicle	:		
Result	:	corrosive	
Classification	:	risk of serious damage to eyes	
Method	:	other: Younger Laboratory method	
Year	:	1978	
GLP	:	no data	
Test substance	:	other TS	
Source	:	Monsanto Europe N.V. Bruxelles	
Test substance	:	45% to 50% sodium MBT content.	
16.04.2003			(28)
Species	:	rabbit	
Concentration	:		
Dose	:		
Exposure time	:		
Comment	:		
Number of animals	:		
Vehicle	:		
Result	:	moderately irritating	
Classification	:	irritating	
Method	:	other: Younger Laboratory method	
Year	:	1987	
GLP	:	yes	
Test substance	:	other TS	
Source	:	Monsanto Europe N.V. Bruxelles	
Test substance	:	22% substance content.	
01.06.1994			(29)

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Date 18.06.2003

Species : rabbit
Concentration :
Dose :
Exposure time :
Comment :
Number of animals :
Vehicle :
Result : corrosive
Classification : risk of serious damage to eyes
Method : other: Acute Eye Irritation
Year : 1975
GLP : no data
Test substance : no data

Source : Monsanto Europe N.V. Bruxelles
23.05.1994

(35)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic
Species : rat
Sex :
Strain : Sprague-Dawley
Route of admin. : dermal
Exposure period : 91 days
Frequency of treatm. : daily
Post exposure period : none
Doses : 0, 200, 1000, 2000 mg/kg bw
Control group : yes
NOEL : 200 mg/kg bw
Method : EPA OPPTS 870.3250
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : The NOEL was 200 mg/kg bw. The LOEL was 1000 mg/kg/day based on statistically significant increase in liver weights at 1000 and 2000 mg/kg/day in female rats. No other adverse effects due to treatment were found.

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint
14.05.2003

(50)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538
Test concentration : 0.001, 0.01, 0.1, 1.0 or 5.0 ul/plate
Cycotoxic concentr. : With metabolic activation: 5.0 ul/plate; Without metabolic activation: 5.0 ul/plate
Metabolic activation : with and without
Result : negative
Method : other: Ames Mutagenicity Plate Test (Overlay Method) 1975
Year :

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GLP	:	yes	
Test substance	:	as prescribed by 1.1 - 1.4	
Result	:	The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.	
Test condition	:	The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The Salmonella typhimurium strains used for this experiment were obtained from Dr. Bruce Ames. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. Chemicals used as positive controls for the non-activation assays were methylnitrosoguanidine (MNNG), 2-nitrofluorene (NF) and quinacrine mustard (QM). Positive control chemicals used for the activation assays were 2-anthramine (ANTH), 2-acetylaminofluorene (AAF) and 8-aminoquinoline (AMQ). Dimethylsulfoxide (DMSO) was used as the solvent and the solvent control at 2.5%/plate.	
Reliability	:	(1) valid without restriction GLP guideline study	
Flag 16.04.2003	:	Critical study for SIDS endpoint	(51)
Type	:	Mammalian cell gene mutation assay	
System of testing	:	Balb/3T3 cells	
Test concentration	:	78.0 to 13.0 nl/ml	
Cycotoxic concentr.	:	78.0 nl/ml	
Metabolic activation	:	without	
Result	:	negative	
Method	:	Directive 87/302/EEC, part B, p. 73	
Year	:	1982	
GLP	:	no data	
Test substance	:	other TS: NACAP; purity not noted	
Method	:	Directive 87/302/EEC, Part B Mutagenicity - in vitro mammalian cell transformation tests, 1982, and Kakunaga, T., A Quantitative System for Assay of Malignant Transformation by Chemical Carcinogens using a Clone Derived from BALB/3T3, 1973	
Result	:	The test substance did not induce the appearance of a significant number of transformed foci over the concentration range of 78.0 to 13.0 nl/ml. Therefore the test substance is considered to be inactive in the Balb/3T3 in vitro Transformation Assay.	
Test condition	:	The I(13) BALB/3T3 mouse cell clones for this study were obtained from Dr. Kakunaga of the National Cancer Institute. Further subclones, selected for low spontaneous frequencies of foci formation, were used for the assay. DMSO was used for the solvent and the solvent (negative) control. A known carcinogen, 3-methylcholanthrene was used as the positive control. A preliminary cytotoxicity test determined the concentrations selected for the transformation assay (78.0 ul/ml - 13.0 ul/ml, corresponding to a survival range of 20-90%).	
Reliability	:	(1) valid without restriction Guideline study	
Flag 14.05.2003	:	Critical study for SIDS endpoint	(52)
Type	:	Yeast gene mutation assay	
System of testing	:	Saccharomyces cerevisiae D4	
Test concentration	:	0.001, 0.01, 0.1, 1.0 or 5.0 ul/plate	

5. Toxicity

Id 2492-26-4

Date 18.06.2003

Cycotoxic concentr. : With metabolic activation: 5.0 ul/plate; Without metabolic activation. 5.0 ul/plate
Metabolic activation : with and without
Result : negative
Method : other: Ames Mutagenicity Plate Test (Overlay Method) 1975
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.

Test condition : The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. The chemical used as positive control for the non-activation assay was methylnitrosoguanidine (MNNG) at 10 ug/plate. Positive control chemical used for the activation assay was DMNA at 100 micromoles/plate. Dimethylsulfoxide (DMSO) at 2.5%/plate was used as the solvent and the solvent control.

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint

14.05.2003

(51)

Type : Ames test
System of testing : Salmonella typhimurium
Test concentration :
Cycotoxic concentr. :
Metabolic activation :
Result : ambiguous
Method : other
Year : 1983
GLP : no data
Test substance : no data

Remark : weakly positive, no other data available

Source : Monsanto Europe N.V. Bruxelles

14.05.2003

(53)

Type : Unscheduled DNA synthesis
System of testing : rat primary hepatocytes
Test concentration :
Cycotoxic concentr. :
Metabolic activation :
Result : negative
Method : EPA OTS 798.5550
Year :
GLP :
Test substance : other TS: 2-mercaptobenzothiazole (CAS# 149-30-4)

Remark : Sodium MBT is similar in toxicity to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thizoles category of chemicals.

Reliability : (1) valid without restriction

14.05.2003

(54)

5. Toxicity

Id 2492-26-4

Date 18.06.2003

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Micronucleus assay
Species : mouse
Sex :
Strain :
Route of admin. :
Exposure period :
Doses :
Result : negative
Method :
Year :
GLP :
Test substance : **other TS: 2-mercaptobenzothiazole (CAS# 149-30-4)**

Remark : Sodium MBT is similar in toxicity to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thizoles category of chemicals.

Reliability : (1) valid without restriction
14.05.2003 (55)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study
Species : rat
Sex : male/female
Strain : other: CrI: CD COBS BR
Route of admin. : oral feed
Exposure period :
Frequency of treatm. :
Premating exposure period :
 Male :
 Female :
Duration of test :
No. of generation :
studies :
Doses : 0, 2500, 8750, 15000 ppm (0, 194, 695, 1195 mg/kg/day)
Control group :
Method : EPA OPPTS 870.3800
Year :
GLP :
Test substance : **other TS: 2-mercaptobenzothiazole (CAS# 149-30-4)**

Remark : Sodium MBT is similar in toxicity to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thizoles category of chemicals.

Result : Reproductive/systemic NOEL = 2500 ppm (194 mg/kg/day), LOEL = 8750 ppm (695 mg/kg/day) based on decrease in body weight.

Reliability : (1) valid without restriction
14.05.2003 (56)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley

5. Toxicity

Id 2492-26-4

Date 18.06.2003

Route of admin. : gavage
Exposure period : Gestation days 6 -15
Frequency of treatm. : daily
Duration of test :
Doses : 0, 300, 1200, 1800 mg/kg/day
Control group : yes
NOAEL maternal tox. : 300 mg/kg bw
NOAEL teratogen. : 1200 - mg/kg bw
Method : EPA OPPTS 870.3700
Year :
GLP :
Test substance : **other TS: 2-mercaptobenzothiazole (CAS# 149-30-4)**

Remark : Sodium MBT is similar in toxicity to 2-MBT, this study on 2-MBT is used to fill this endpoint in the Benzothiazole-based thizoles category of chemicals.

Result : The LOEL for maternal toxicity was 1200 mg/kg/day due to hair loss, increased salivation and urine staining. The LOEL for developmental toxicity was 1800 mg/kg/day due to greater post-implantation loss.

Reliability : (1) valid without restriction
14.05.2003 (57)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6. Analyt. Meth. for Detection and Identification

Id 2492-26-4
Date 18.06.2003

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 2492-26-4
Date 18.06.2003

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8. Meas. Nec. to Prot. Man, Animals, Environment

Id 2492-26-4
Date 18.06.2003

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

Id 2492-26-4

Date 18.06.2003

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9. References

Id 2492-26-4

Date 18.06.2003

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- (31) R.T. Vanderbilt Co. (1975). Material Safety Data Sheet - Sodium 2-Mercaptobenzothiazole, Norwalk, CT. Cited in: Syracuse Research Corporation (1976): NTIS/PB 256662
- (32) American Cyanamid Co. (1965). Toxicity data on sodium MBT solution. Report No. 65-1. Cited in: Technical Support Document, Contract No. 68-02-4209, task 6, Syracuse Research Corporation (1985)
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9. References

Id 2492-26-4

Date 18.06.2003

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10. Summary and Evaluation

Id 2492-26-4
Date 18.06.2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical : ID: 95-16-9
CAS No. : 95-16-9
EINECS Name : benzothiazole
EC No. : 202-396-2
Molecular Weight : 135.2
Molecular Formula : C7H5NS

Producer related part
Company : Bayer Corporation
Creation date : 03.06.2003

Substance related part
Company : Bayer Corporation
Creation date : 03.06.2003

Status :
Memo : American Chemistry Council, Rubber and Plastic Additives Panel,
Non-sponsored chemical – used for data purposes only

Printing date : 19.06.2003
Revision date :
Date of last update : 18.06.2003

Number of pages : 47

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. General Information

Id 95-16-9

Date 19.06.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : cooperating company
Name : Flexsys America L.P.
Contact person :
Date :
Street : 260 Springside Drive
Town : 44333-0444 Akron, OH
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

Source : American Chemistry Council, Rubber and Plastic Additives (RAPA) Panel
03.06.2003

Type :
Name : Bayer Antwerpen N.V.
Contact person :
Date :
Street : Haven 507, Scheldelaan 420
Town : Antwerpen
Country : Belgium
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type :
Name : Flexsys S.A.
Contact person :
Date :
Street : Woluwe Garden, Woluwedal 24
Town : B-1932 St.-Stevens-Woluwe
Country : Netherlands
Phone : +32 (2) 714 32 25
Telefax : +32 (2) 714 32 35
Telex :
Cedex :
Email :
Homepage :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type :
Name : GENERAL QUIMICA, S.A.
Contact person :
Date :
Street : Km.4 Ctra. de Miranda a Puentelarra
Town : 01213 LANTARON COMUNION (ALAVA)
Country : Spain
Phone : 947-31 01 45

1. General Information

Id 95-16-9

Date 19.06.2003

Telefax : 947-31 38 88
Telex : 39531
Cedex :
Email :
Homepage :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

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 :
Smiles Code : c1ccc2ncsc2c1
Molecular formula : C7-H5-N-S
Molecular weight : 135.18
Petrol class :

03.06.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : liquid
Purity : 88 - 98 % v/v
Colour : Yellow to brown
Odour :

03.06.2003

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

Source : Bayer AG Leverkusen
08.07.1994

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1-Thia-3-azaindene

Source : Flexsys S.A. St.-Stevens-Woluwe
Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
02.02.1999

Benzosulfonazole

Source : Flexsys S.A. St.-Stevens-Woluwe
Bayer Antwerpen N.V. Antwerpen
GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)

1. General Information

Id 95-16-9

Date 19.06.2003

02.02.1999 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Benzothiazol

Source : Bayer AG Leverkusen
08.07.1994

Benzothiazole (6CI, 8CI, 9CI)

Source : Flexsys S.A. St.-Stevens-Woluwe
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
02.02.1999

BT

03.06.2003

BTH

Source : Flexsys S.A. St.-Stevens-Woluwe
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
02.02.1999

Rubator BT

Source : GENERAL QUIMICA, S.A. LANTARON COMUNION (ALAVA)
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
06.05.1998

Vangard® BT

Source : American Chemistry Council, Rubber and Plastic Additives (RAPA) Panel
03.06.2003

1.3 IMPURITIES

Purity :
CAS-No : 120-75-2
EC-No : 204-423-3
EINECS-Name : 2-methylbenzothiazole
Molecular formula :
Value : .5 - 5 % v/v

Source : American Chemistry Council, Rubber and Plastic Additives (RAPA) Panel
03.06.2003

Purity :
CAS-No : 62-53-3
EC-No : 200-539-3
EINECS-Name : aniline
Molecular formula :
Value : 0 - 4 % v/v

Source : American Chemistry Council, Rubber and Plastic Additives (RAPA) Panel
03.06.2003

Purity :
CAS-No : 108-88-3
EC-No : 203-625-9
EINECS-Name : toluene
Molecular formula :

1. General Information

Id 95-16-9
Date 19.06.2003

Value : 0 - 1 % v/v

Source : American Chemistry Council, Rubber and Plastic Additives (RAPA) Panel
03.06.2003

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : type
Category : Non dispersive use

03.06.2003

Type of use : type
Category : Use in closed system

03.06.2003

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

03.06.2003

Type of use : use
Category : Intermediates

03.06.2003

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

Type : TSCA
Additional information :

03.06.2003

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1. General Information

Id 95-16-9
Date 19.06.2003

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 95-16-9

Date 19.06.2003

2.1 MELTING POINT

Value	:	2 - °C
Decomposition	:	no, at - °C
Sublimation	:	no
Method	:	other: FF88.2-1, Determination of Crystallizing Point of Organic Compounds, 1998
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Flexsys Standard Method FF88.2-1, Determination of Crystallizing Point of Organic Compounds, January 09, 1988.
Reliability	:	(1) valid without restriction GLP Guideline study
Flag 03.06.2003	:	Critical study for SIDS endpoint
Value	:	2 - °C
Sublimation	:	
Method	:	other: Handbook value
Year	:	
GLP	:	no data
Test substance	:	other TS: benzothiazole (CAS# 95-16-9); purity not noted
Reliability	:	(2) valid with restrictions Data from Handbook or collection of data
Flag 03.06.2003	:	Critical study for SIDS endpoint

(1)

2.2 BOILING POINT

Value	:	231 - °C at 1013 hPa
Decomposition	:	no
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Measured boiling point for benzothiazole distillation from the Flexsys Standard Manufacturing Process Manual for MBT Solution.
Reliability	:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment.
Flag 03.06.2003	:	Critical study for SIDS endpoint
Value	:	231 - °C at
Decomposition	:	
Method	:	other: Handbook value
Year	:	
GLP	:	no data
Test substance	:	other TS: benzothiazole (CAS# 95-16-9); purity not noted
Reliability	:	(2) valid with restrictions Data from Handbook or collection of data
Flag 03.06.2003	:	Critical study for SIDS endpoint

(2)

(1)

2.3 DENSITY

Type	:	density
Value	:	ca. 1.246 - at 22 °C

2. Physico-Chemical Data

Id 95-16-9

Date 19.06.2003

Method : other: FF97.4/ASTM D891-94, 1997
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : Specific Gravity of Liquids by Hydrometers. Hydrometers must meet ASTM E100 specifications.

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint

03.06.2003

(3)

Type : density

Value : 1.246 - at 20 °C

Method : other: Handbook value

Year :

GLP : no data

Test substance : other TS: benzothiazole (CAS# 95-16-9); purity not noted

Reliability : (2) valid with restrictions
Data from Handbook or collection of data

Flag : Critical study for SIDS endpoint

03.06.2003

(1)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .01866 - hPa at 25 °C

Decomposition :

Method : other (measured)

Year :

GLP : yes

Test substance : as prescribed by 1.1 - 1.4

Remark : Vapor pressure for benzothiazole from the Flexsys Standard Manufacturing Process Manual for MBT Solution

Result : 3.866 hPa at 80°C
10.799 hPa at 100°C
89.326 hPa at 150°C
449.295 hPa at 200°C
1006.581 hPa at 230°C

Reliability : (1) valid without restriction
GLP study

Flag : Critical study for SIDS endpoint

04.06.2003

(2)

2.5 PARTITION COEFFICIENT

Partition coefficient :

Log pow : 1.94 - at 25 °C

pH value : -

Method : other (measured): GC Method for Pow, 1978

Year :

GLP : no

Test substance :

Method : 1% and .01% solutions in 100 ml n-Octanol added to 500 ml water. Shaken for 48 hours, equilibration for several days. Equilibration performed in the dark to preclude photodegradation. Analysis via GC to determine Pow; Pow = 88 +/- 4.

2. Physico-Chemical Data

Id 95-16-9

Date 19.06.2003

Remark : Good agreement with calculation method, SRC LogKow (KowWin) Program 1995.
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.
Flag : Critical study for SIDS endpoint
04.06.2003 (4)

Partition coefficient :
Log pow : 2.17 - at 25 °C
pH value : -
Method : other (calculated): EPIWIN/KOWWIN v1.66
Year :
GLP : no
Test substance : other TS: molecular structure of benzothiazole (CAS # 95-16-9)

Remark : Estimation method based on molecular structure fragments
Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
04.06.2003 (5)

Partition coefficient :
Log pow : 2 - at °C
pH value : -
Method : other (calculated): Leo, Hansch: Leo, A. CLOGP-3.63 (1991) Daylight, Chemical Information Systems Inc. Irvine, CA, USA
Year :
GLP :
Test substance :

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
30.05.1995 (6)

Partition coefficient :
Log pow : 2.01 - at °C
pH value : -
Method : other (measured)
Year :
GLP :
Test substance :

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
08.07.1994 (7)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : 3590 - 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: Saturated Solution / Solvent Extraction / GC Analysis, 1978
Year :
GLP : no data

2. Physico-Chemical Data

Id 95-16-9

Date 19.06.2003

Test substance	:	as prescribed by 1.1 - 1.4	
Method	:	The aqueous solubility was determined by adding 1g of the test compound and 500ml purified water to a 1 liter glass bottle with an aluminium foil lined cap. The solution was mixed with a magnetic stirrer for several days to produce a saturated solution. Equilibration was performed in the dark to preclude photodegradation. Stirring was stopped one hour before sampling to permit phase separation. The aqueous layer was extracted with methylene chloride and analyzed via gas chromatography.	
Reliability	:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment.	
Flag 04.06.2003	:	Critical study for SIDS endpoint	(4)
Solubility in Value	:	ca. 3 - g/l at 20 °C	
pH value concentration	:	- at °C	
Temperature effects	:		
Examine different pol.	:		
pKa	:	at 25 °C	
Description	:		
Stable	:		
Source 08.07.1994	:	Bayer Antwerpen N.V. Antwerpen EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	(8)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	115.6 °C	
Type	:	open cup	
Method	:	other: ASTM D 92, 1977	
Year	:		
GLP	:	no data	
Test substance	:	as prescribed by 1.1 - 1.4	
Reliability 04.06.2003	:	(1) valid without restriction Guideline study	(9)
Value	:	ca. 107 °C	
Type	:		
Method	:	other: DIN 51758	
Year	:		
GLP	:		
Test substance	:		
Source 08.07.1994	:	Bayer Antwerpen N.V. Antwerpen EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	(8)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2. Physico-Chemical Data

Id 95-16-9

Date 19.06.2003

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

Memo : Henry's Law Constant

Method : ABC Protocol A-8301, Determination of Air-Water Henry's Law Constant, 1984, and Mackay, D. et al., Determination of Henry's Law Constants for Hydrophobic Pollutants, 1979
GLP Study.

Remark : The Henry's Law constant of the test substance in deionized water was determined as the mean of duplicate test systems to be 3.6×10^{-3} 1-atm/mole with a standard deviation of 0.07×10^{-3} .

Result : 3.6×10^{-3} atm-m³/mole

Reliability : (1) valid without restriction
GLP study

04.06.2003

(10)

3. Environmental Fate and Pathways

Id 95-16-9

Date 19.06.2003

3.1.1 PHOTODEGRADATION

Type : water
Light source : Sun light
Light spectrum : 250 - nm
Relative intensity : - based on intensity of sunlight
Conc. of substance : 1.018 mg/l at 26 °C
DIRECT PHOTOLYSIS
Halflife t1/2 : 110 - day(s)
Degradation : 100 - % after 170 day(s)
Quantum yield :
Deg. product :
Method : other (measured): Method similar to ASTM Draft Method No. 6, ASTM E35.24, Subcommittee, Aqueous Photolysis Task Group, 1980
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Both direct and sensitized photolysis rates were not significant, with half-lives of > 100 days observed, indicating that the test substance is very stable chemically in water. Samples were analyzed via direct aqueous injection into an HPLC equipped with a variable wavelength detector.

Result : Half life:
110 days in Milli-Q (purified) water
143 days in Mississippi River water
Degradation:
170 days in Milli-Q (purified) water
485 days in Mississippi River water

Test substance : purity: >94%
Reliability : (1) valid without restriction
Guideline study
Flag : Critical study for SIDS endpoint

18.06.2003

(11)

Type : air
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 156000000 molecule/cm³
Rate constant : .000000000007 cm³/(molecule*sec)
Degradation : 50 - % after 18.3 hour(s)
Deg. product :
Method : other (calculated): AOP Program v1.90, 2001
Year :
GLP : no
Test substance : other TS: molecular structure of benzothiazole (CAS# 95-16-9)

Flag : Accepted calculation method
Critical study for SIDS endpoint

18.06.2003

(12)

Type : air
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
Deg. product :
Method : other (calculated): acc. to Atkinson: SRC-AOP for Microsoft Windows
Year :
GLP :

3. Environmental Fate and Pathways

Id 95-16-9

Date 19.06.2003

Test substance : other TS: molecular structure of benzothiazole (CAS# 95-16-9)

Remark : Sensitizer: OH
Conc. of Sensitizer: 0.5E6 OH/cm3
Rate Constant: 7.0E-12 cm3/molecule x sec
Half life time: 4.584 d

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
Accepted calculation method

04.06.2003 (13)

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: EPIWIN v3.10

Year :

Remark : Calculations based on user input values of water solubility, vapor pressure, Henry LC, Log Kow, melt point and boiling point.

Result :

	Mass Amount (%)	Half-life (hrs)	Emissions (kg/hr)
Air	23.3	36.7	1000
Water	56.4	360	1000
Soil	20.1	360	1000
Sediment	0.16	1.44E+3	0

Persistence time estimated at 114 Hours

Reliability : (2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint

04.06.2003 (12)

Type : volatility

Media : water - air

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: Estimation Method, 1990

Year :

Remark : Model river = 1 m deep flowing at 1 m/sec and wind velocity of 3 m/sec.
Model lake = 1 m deep flowing at 0.05 m/sec and wind velocity of 0.5 m/sec

Result : Volatilization half-life from model river: 1.376 hours
Volatilization half-life from model lake: 112.5 hours
Volatilization Constant from water: 3.6 x 10⁻³ atm-m³/mole

Reliability : (2) valid with restrictions

3. Environmental Fate and Pathways

Id 95-16-9

Date 19.06.2003

Flag : Accepted calculation method
04.06.2003 : Critical study for SIDS endpoint (14)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 20.4 mg/l related to Test substance related to
Contact time :
Degradation : < 24 - (\pm) % after 36 day(s)
Result :
Deg. product :
Method : other: ASTM Proposed Standard Practice for the Determination of the Ultimate Biodegradability of Organic Chemicals, Draft No. 3, ASTM E35.24, Shake Flask CO₂ Procedure, 1980
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Triplicate flasks produced 0-24% theoretical CO₂, suggesting that the microbial population was very sensitive to small changes in system parameters. Values in this range usually indicate that the test substance is resistant to biodegradation, that the test compound undergoes primary biodegradation and possibly partial mineralization to a more resistant metabolite, or that the test compound is mineralized to CO₂, but at a very slow rate.

Test condition : Medium: soil, raw sewage and activated sludge mixed liquor
Test substance : purity: >94%
Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint
18.06.2003 (15)

Type : aerobic
Inoculum : other: sludge samplings from different sewage plants, rivers, bays and a lake
Concentration : 100 mg/l related to Test substance related to
Contact time :
Degradation : 0 - (\pm) % after 28 day(s)
Result : under test conditions no biodegradation observed
Deg. product :
Method : other:
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : "Biodegradation test of chemical substance by microorganisms etc." stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, 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).

Remark : related to BOD
sludge conc.: 30 mg/l

3. Environmental Fate and Pathways

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Date 19.06.2003

Reliability	:	(1) valid without restriction Guideline study	
Flag 04.06.2003	:	Critical study for SIDS endpoint	(16)
Type	:	aerobic	
Inoculum	:	predominantly domestic sewage	
Concentration	:	.8 mg/l related to related to	
Contact time	:		
Degradation	:	> 65 - (\pm) % after 21 day(s)	
Result	:	inherently biodegradable	
Deg. product	:		
Method	:	OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"	
Year	:	1984	
GLP	:	no	
Test substance	:	as prescribed by 1.1 - 1.4	
Source	:	Bayer Antwerpen N.V. Antwerpen EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
Reliability	:	(1) valid without restriction Guideline study	
Flag 04.06.2003	:	Critical study for SIDS endpoint	(17)

3.6 BOD5, COD OR BOD5/COD RATIO

Remark	:	ThOD: 2553 mg/g COD: 2157 mg/g	
Source 11.08.1994	:	Bayer Antwerpen N.V. Antwerpen EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	(17)
Remark	:	ThOD: 2553 mg/g COD: 2157 mg/g	
Source 11.08.1994	:	Bayer AG Leverkusen	(17)

3.7 BIOACCUMULATION

Species	:	Cyprinus carpio (Fish, fresh water)	
Exposure period	:	42 day(s) at °C	
Concentration	:	.2 mg/l	
BCF	:	2.1 - 5.1	
Elimination	:		
Method	:	other: MITI Bioaccumulation test of chemical substance in fish and shellfish, 1974. Corresponds to OECD 305C, Bioaccumulation: Degree of Bioconcentration in Fish, 1981	
Year	:		
GLP	:	no data	
Test substance	:	as prescribed by 1.1 - 1.4	
Result	:	Conc. (mg/l) BCF 0.2 2.1-5.1 0.02 < 4.1-7.5 % lipid, average 4.0	
Reliability 04.06.2003	:	(1) valid without restriction Guideline study	(16)

3. Environmental Fate and Pathways

Id

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Species : other
Exposure period : at °C
Concentration :
BCF : 14 - 16
Elimination :
Method : other: Calculation, Neely, et. al., 1974
Year :
GLP : no
Test substance :

Remark : Calculation from measured octanol/water partition coefficient, $P_{ow} = 88$.
Reliability : (2) valid with restrictions
Accepted calculation method

04.06.2003

(4)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 95-16-9

Date 19.06.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : flow through
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : 8.1 -
Limit test :
Analytical monitoring Method : yes
: other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians, 1975
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : The test was performed under continuous flow conditions using a Mount-Brungs diluter. It was conducted in 19-liter glass aquaria, with 10 fish/replicate. Flow rate was set to provide five tank volumes/day. Juvenile trout, obtained from Mt. Lassen Trout Farm, were maintained at SRI for at least two weeks prior to testing. Average fish length was 4.56 cm, and weight was 0.86 g. Fish were fed a daily ration (5% of body weight) of frozen brine shrimp. The stock solution was prepared by adding 50 grams of the test compound to 200 liters of diluent water and stirring for 48 hours. Nominal test concentrations were 0.0, 1.5, 3.1, 6.2, 12.5 and 25.0 mg/l. The test was terminated after 14 days of exposure. The LC50 values and 95% confidence limits were calculated by using a computerized program that employed the binomial method and the probit test with Berkson's Adjustment.

Result : LC50 (24h) = >22.4 mg/l
LC50 (96h) = 8.1 mg/l
LC50 (336h) = 5.6 mg/l (14 days)

Test condition : Dissolved oxygen (DO), pH, temperature and chemical concentrations were measured routinely, alternating between the replicates. DO ranged from 9.4-10.8 mg/l, pH from 6.8 to 8.2, temperature between 13.0 and 14.0°C. Hardness, as CaCO₃, was 28 mg/l, alkalinity was 29 mg/l, and acidity was <5.0 mg/l. Test chemical concentrations were determined by an internal standard HPLC method. Measured concentrations of the test chemical were 0, 1.6, 4.4, 8.1, 14.9 and 22.9 mg/l.

Test substance : purity: 96%.

Conclusion : The mortality data indicate that the test compound has a fairly high acute toxicity to rainbow trout at levels quite a bit less than its solubility limits. In addition, the pattern of continuing mortality throughout the test period suggests that this compound is cumulatively toxic over longer exposure periods.

Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint

18.06.2003

(18)

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : 18 -
LC50 : 47 -
Limit test :
Analytical monitoring Method : no
: other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians (1972).

Year :

4. Ecotoxicity

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Date 19.06.2003

GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	<p>Test fish were obtained from Fattig Fish Hatchery in Brady, Nebraska. Test fish were held in culture tanks on a 16-hour daylight photoperiod and observed for at least 14 days prior to testing. A daily record of fish observations was maintained during the holding period, during which time the fish were fed a standard diet of commercial fish food until 48 hours prior to testing, when feeding was stopped.</p> <p>Test fish had a mean weight of 0.15 g and a mean standard length of 21.7 mm. The test was conducted in 5-gallon glass vessels containing 15 liters of laboratory well water. Test fish were acclimated to the dilution water and test temperature, and held without food for 48 hours prior to testing. Nanograde Acetone was used to prepare the test solutions and as the solvent control. Test concentrations were 0, 10, 18, 32, 56 and 100 mg/l for the test compound.</p> <p>Fish were placed in the testing vessels within 30 minutes of the addition of the test material aliquots. All groups were observed once every 24 hours for mortality and abnormal effects. As a quality check, test fish were challenged with Antimycin A.</p> <p>The estimated 96Hr LC50 and 95% confidence limits were within the 95% confidence limits reported in the literature, indicating that the fish were in good condition. These values were obtained by employing the statistical methods described by Litchfield and Wilcoxon (A Simplified Method for Evaluating Dose-Effect Experiments, 1949) or Stephan (methods for calculating an LC50, 1977).</p>
Result	:	<p>LC50 (24h) = 47 mg/l LC50 (48h) = 47 mg/l LC50 (96h) = 47 mg/l NOEC = 18 mg/l LOEC = 32 mg/l</p>
Test condition	:	<p>The 0-hour measured control water parameters of this dilution water were dissolved oxygen 9.3 ppm, hardness (CaCO₃) of 255 ppm and pH 8.2. The test vessels were kept in a water bath at 22°C. Dissolved oxygen values and pH ranges were monitored during the testing and remained within acceptable limits of 40-100% saturation for dissolved oxygen and pH value consistent with control. The ammonia concentration was below the toxic limit. Water hardness (CaCO₃) was 255 ppm.</p>
Test substance	:	purity: >94%
Reliability	:	<p>(1) valid without restriction GLP Guideline study</p>
Flag	:	Critical study for SIDS endpoint
04.06.2003		(19)
Type	:	static
Species	:	Cyprinodon variegatus (Fish, estuary, marine)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	< 10 -
LC50	:	36 -
LOEC	:	10 -
Limit test	:	
Analytical monitoring	:	no
Method	:	other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians (1972).
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	<p>Test fish were obtained from Multiaqua Culture System in Amagansett, New York. Test fish were held in culture tanks on a 16-hour daylight photoperiod and observed for at least 14 days prior to testing. A daily</p>

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record of fish observations was maintained during the holding period, during which time the fish were fed a mixed diet of brine shrimp nauplii and Tetramin® fish food daily until 48 hours prior to testing, when feeding was stopped. Test fish had a mean weight of 0.32 g and a mean standard length of 21 mm. The test was conducted in 5-gallon glass vessels containing 15 liters of reconstituted salt water and deionized water. Test fish were acclimated to the dilution water and test temperature, and held without food for 48 hours prior to testing.

A 96-hour range-finding study preceded the definitive study. Test concentrations were 0, 10, 18, 32, 56 and 100 mg/l for the test compound. 1.5 ml of triethylene glycol was added to sample weights before mixing in the test chambers. Test concentrations were obtained by transferring appropriate weights of the test compound directly to the test chambers. Also included were a dilution water control and a solvent control. The solvent control received an aliquot of 1.5 ml of triethylene glycol. Fish were placed in the testing vessels within 30 minutes of the addition of the test material aliquots. All groups were observed once every 24 hours for mortality and abnormal effects.

Statistical analysis of the concentration vs. effect data was obtained by employing a computerized LC50 program developed by Stephan et al. This program calculated the LC50 statistic and its 95% confidence limits using the binomial, the moving average and the probit tests.

Result	:	LC50 (24h) = 70 mg/l LC50 (48h) = 64 mg/l LC50 (96h) = 36 mg/l NOEC = <10 mg/l LOEC = 10 mg/l
Test condition	:	The 0-hour measured control water parameters of this dilution water were dissolved oxygen 6.9 mg/l (corrected for salinity), salinity of 20 ppt, hardness (CaCO ₃) of 255-275 ppm and pH 8.1. The test vessels were kept in a water bath at 22°C. Dissolved oxygen values and pH ranges were monitored during the testing and remained within acceptable limits of 95-75% saturation for dissolved oxygen and pH 8.1-7.6.
Test substance	:	purity: 99%
Reliability	:	(1) valid without restriction GLP Guideline study
Flag 18.06.2003	:	Critical study for SIDS endpoint
		(20)
Type	:	static
Species	:	Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	187 -
LC50	:	26 -
Limit test	:	
Analytical monitoring	:	no
Method	:	other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians (1972)
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The test material, in reagent-grade acetone, was introduced into 15 liters of diluent water in all-glass vessels. Test concentrations were 0, 18, 24, 32, 42 or 56 mg/l for the test compound. Ten rainbow trout, standard length 3.7 cm, were added to each test vessel. The test fish were not fed for 48 hours prior to testing, nor during the exposure period. Observations and mortality counts were made every 24 hours during a 96-hour period following the initiation of exposure. Test concentrations and observed percentage mortality were converted to logarithms and probits, respectively, and these

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values were utilized in a least squares regression analysis. The LC50 values and the 95% confidence intervals were calculated from the regression equation.

Result : LC50 (24h) = 35 mg/l
LC50 (48h) = 30 mg/l
LC50 (96h) = 26 mg/l
NOEC = 18 mg/l
LOEC = 24 mg/l

Test condition : No aeration was provided during the test. Temperature was maintained at 12°C. Dissolved oxygen content ranged from 9.9 mg/l (93% of saturation) at the beginning of the test, to 2.0 mg/l (19% of saturation) at the end of the exposure period. Beginning pH was 7.4; ending pH was 6.8. Water hardness (CaCO₃) was 255 ppm.

Test substance : purity: >94%

Reliability : (1) valid without restriction
Guideline study

04.06.2003 (21)

Type : static

Species : Lepomis macrochirus (Fish, fresh water)

Exposure period : 96 hour(s)

Unit : mg/l

NOEC : 10 -

LC50 : 18 -

Limit test :

Analytical monitoring Method : no
other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians (1972).

Year :

GLP : no

Test substance : as prescribed by 1.1 - 1.4

Method : The test material, in reagent-grade acetone, was introduced into 15 liters of diluent water in all-glass vessels. Test concentrations were 0, 10, 14, 18, 24, 32, 42, 56 and 75 mg/l for the test compound. Ten bluegill, standard length 3.8 cm, were added to each test vessel. The test fish were not fed for 48 hours prior to testing, nor during the exposure period. Observations and mortality counts were made every 24 hours during a 96-hour period following the initiation of exposure. Test concentrations and observed percentage mortality were converted to logarithms and probits, respectively, and these values were utilized in a least squares regression analysis. The LC50 values and the 95% confidence intervals were calculated from the regression equation.

Result : LC50 (24h) = >56<75 mg/l
LC50 (48h) = 44 mg/l
LC50 (96h) = 18 mg/l
NOEC = 10 mg/l
LOEC = 14 mg/l

Test condition : No aeration was provided during the test. Temperature was maintained at 22°C. Dissolved oxygen content ranged from 9.1 mg/l (103% of saturation) at the beginning of the test, to 0.2 mg/l (2% of saturation) at the end of the exposure period. Beginning pH was 7.3; ending pH was 6.7. Water hardness (CaCO₃) was 255 ppm.

Test substance : purity: >94%

Reliability : (1) valid without restriction
Guideline study

04.06.2003 (21)

Type : static

Species : Brachydanio rerio (Fish, fresh water)

Exposure period : 96 hour(s)

Unit : mg/l

4. Ecotoxicity

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LC0 : 65.5 -
LC100 : 66 -
Limit test :
Analytical monitoring : no
Method : other: DIN 38 412, Teil 15: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische, Fischtest (L 15) (Juni 1982)
Year : 1984
GLP : no
Test substance :

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
04.06.2003 (17)

Type : static
Species : *Oryzias latipes* (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : 87.2 -
Limit test :
Analytical monitoring : no data
Method : other: Japanese Industrial Standard (JIS K 0102-1986-71) "Testing methods for industrial waste water"
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Test substance : no data on purity
Reliability : (1) valid without restriction
Guideline study
04.06.2003 (16)

Type : flow through
Species : *Pimephales promelas* (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : 64 -
Limit test :
Analytical monitoring : yes
Method :
Year : 1989
GLP :
Test substance : other TS: purity > 96 %

Remark : 96h-EC50: 60.7 mg/l
Analytical monitoring: GLC
Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
04.06.2003 (22)

Type :
Species : *Oryzias latipes* (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : 110 -
Method :
Year :
GLP : no
Test substance :

Remark : QSAR calculation
Source : Bayer Antwerpen N.V. Antwerpen

4. Ecotoxicity

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EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

(23)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	5.6 -
EC50	:	20 -
Analytical monitoring	:	no
Method	:	other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians, EPA-660/3-75-009, 1975
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	<p>The Daphnia magna used in the test were cultured at the ABC facilities. The adult Daphnia were fed the algae Selenastrum capricornutum at least every three days prior to testing and supplemented with a suspension of trout chow. The bioassay was conducted in 500-ml glass beakers containing 250 ml of ABC well water.</p> <p>An initial range-finding experiment was carried out to determine the exposure concentrations for the definitive test. Water was used as the solvent for the test solutions and as the control. Ten daphnia (first instar less than 18 hours old) were selected for each of the test concentrations (0, 1.0, 3.2, 5.6, 10, 32 and 56 mg/l) in duplicate. Daphnia in all concentrations were observed once every 24 hours for mortality and abnormal effects. LC50 and 95% CI were calculated employing the technique of Litchfield and Wilcoxon.</p>
Result	:	<p>EC50 (24h) = 40 mg/l EC50 (48h) = 20 mg/l NOEC = 5.6 mg/l</p>
Test condition	:	<p>Water quality parameters were dissolved oxygen (DO) = 8.6 mg/l, pH = 7.7, hardness = 220 mg/l, and alkalinity = 210 mg/l. Vessels were kept at 19°C in a temperature- controlled area. Lighting was maintained at 50-70 foot-candles on a 16-hour daylight photoperiod.</p> <p>DO levels and pH were monitored throughout the testing and were considered adequate and equivalent to those measurements in the control chamber. DO was >7.0 mg/l and pH was 7.9 at the end of the testing.</p>
Test substance	:	purity: 96%.
Reliability	:	(1) valid without restriction GLP Guideline study
Flag	:	Critical study for SIDS endpoint
18.06.2003		(24)
Type	:	static
Species	:	Mysidopsis bahia (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	18 -
EC50	:	34 -
Analytical monitoring	:	no
Method	:	other: EPA Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians, EPA-660/3-75-009, 1975
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The mysid shrimp used in this study were obtained from Multi-Aqua Culture Systems in Amagansett, New York. The mysids received a diet of

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approximately 1 liter of brine shrimp nauplii per day. The static bioassay was conducted in 400 ml glass vessels containing 300 ml of aged saltwater prepared by dissolving the appropriate amount of synthetic seawater salts in aged ABC well water.

The test mysids were fed approximately 2 ml of brine shrimp per vessel per day throughout the duration of the 96-hour test. A 96-hour range-finding study preceded the definitive study. Based on those results, five concentrations of the test compound (10, 18, 32, 56 and 100 mg/l), with ten mysids per concentration, were selected for the definitive bioassay. Also included were a dilution water control and a solvent control chamber. The mysids were added to the test chambers by random assignment within 30 minutes after addition of the test compound. All concentrations were observed once every 24 hours for mortality and abnormal effects. LC50 and 95% CI were calculated employing a computerized program developed by Stephan et al. using the binomial, the moving average and the probit tests.

Result : LC50 (24h) = 40 mg/l
LC50 (48h) = 34 mg/l
LC50 (96h) = 28 mg/l
NOEC = 18 mg/l
LOEC = 32 mg/l

Test condition : The saltwater used for culture and testing was prepared to yield a salinity of between 23-28 o/oo and a pH of 8.1-8.3. The 0-hour measured control water parameters of this dilution water were dissolved oxygen (DO) of 7.0 mg/l, salinity 27 o/oo and pH 8.3. Test vessels were kept in a water bath at 25° C.
Dissolved oxygen levels corrected for salinity and temperature, salinity and pH were monitored throughout the testing and were considered adequate and equivalent to those measurements in the control chamber. DO ranged from 5.6-7.0 mg/l (84-104% saturation @ 25°C), salinity ranged from 27-28, and pH from 8.2-8.3.

Test substance : purity: 99%.
Reliability : (1) valid without restriction
GLP Guideline study

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(25)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : growth rate
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : 10 -
EC50 : 67 -
Limit test :
Analytical monitoring : no
Method : other: US EPA Phytotoxicity Method - Algal Assay Procedure: Bottle Test (1971)
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : The test algae were obtained from the US EPA Environmental Research Laboratory in Corvallis, Oregon. Beginning cell numbers in the test flasks were 2.0×10^4 cells/ml. Cultures were incubated at 24°C under approximately 4,000 lux illumination. Triplicate cultures were employed for each of the test concentrations and the control. Test containers were 125ml flasks containing 50ml of test medium. Concentrations for the definitive test were based on the results of a 96-hr range-finding study. These concentrations were 0, 6, 10, 32, 56 and 100 mg/ml. Test concentrations were dissolved in reagent-grade acetone. The solvent control was 0.05 ml acetone in water.

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Statistical analysis involved converting each test concentration to a logarithm, and the corresponding percentage decrease of in vivo chlorophyll a or cell numbers was converted to a probit (Finny, 1971). The EC50s and 95% confidence limits were then calculated by linear regression. Student's t-test was used to determine whether growth of the solvent control differed from that of the culture medium control. Differences were considered significant at the 95% confidence level.

Result : Decrease in Chlorophyll a:
EC50 (24.h) = >100 mg/l
EC50 (48.h) = >100 mg/l
EC50 (72.h) = 73 mg/l
EC50 (96.h) = 67 mg/l
NOEC = 10 mg/l

Test condition : pH values during the test ranged from 7.8 (0-hour) to 8.1 (96-hour)

Test substance : purity: 99%.

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint
18.06.2003 (26)

Species : Selenastrum capricornutum (Algae)

Endpoint : biomass

Exposure period : 96 hour(s)

Unit : mg/l

NOEC : 10 -

EC50 : 64 -

Limit test :

Analytical monitoring : no

Method : other: US EPA Phytotoxicity Method - Algal Assay Procedure: Bottle Test (1971)

Year :

GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Method : The test algae were obtained from the US EPA Environmental Research Laboratory in Corvallis, Oregon. Beginning cell numbers in the test flasks were 2.0×10^4 cells/ml. Cultures were incubated at 24°C under approximately 4,000 lux illumination. Triplicate cultures were employed for each of the test concentrations and the control. Test containers were 125ml flasks containing 50ml of test medium. Concentrations for the definitive test were based on the results of a 96-hr range-finding study. These concentrations were 0, 6, 10, 32, 56 and 100 mg/ml. Test concentrations were dissolved in reagent-grade acetone. The solvent control was 0.05 ml acetone in water.

Statistical analysis involved converting each test concentration to a logarithm, and the corresponding percentage decrease of in vivo chlorophyll a or cell numbers was converted to a probit (Finny, 1971). The EC50s and 95% confidence limits were then calculated by linear regression. Student's t-test was used to determine whether growth of the solvent control differed from that of the culture medium control. Differences were considered significant at the 95% confidence level.

Test condition : pH values during the test ranged from 7.8 (0-hour) to 8.1 (96-hour)

Test substance : purity: 99%.

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint
05.06.2003 (26)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic

Species : activated sludge

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Exposure period : 3 hour(s)
Unit : mg/l
EC50 : 635 -
EC05 : 216 -
Analytical monitoring : no
Method : ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year : 1990
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
lack of method detail

05.06.2003 (17)

Type : aquatic
Species : Pseudomonas putida (Bacteria)
Exposure period : 30 minute(s)
Unit : mg/l
LC0 : 250 -
Analytical monitoring : no
Method : other: Bewertung toxischer Wasserinhaltsstoffe aus ihrer Inhibitorwirkung auf die Substratoxydation von Pseudomonas Stamm Berlin mit Hilfe polarographischer Sauerstoffmessungen. Robra, K.H.: gwf wasser/abwasser 117(2), 80-86 (1976)
Year : 1984
GLP : no
Test substance : no data

Remark : Study completed in 1984
Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (4) not assignable
data from secondary literature source

05.06.2003 (17)

Type : aquatic
Species : Pseudomonas putida (Bacteria)
Exposure period : 18 hour(s)
Unit : mg/l
LC0 : 50 -
Analytical monitoring : no
Method :
Year : 1990
GLP : no
Test substance :

Remark : Method:
Grenzwerte der Schadwirkung wassergefährdender Stoffe gegen Bakterien (Pseudomonas putida) und Grünalgen (Scenedesmus quadricauda) im Zellvermehrungshemmtest. Bringmann, G.; Kuehn, R.: Z. f. Wasser- und Abwasser-Forschung 10 (3/4), 87-98 (1977)
Study completed in 1990

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (4) not assignable
data from secondary literature source

05.06.2003 (17)

Type : aquatic

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Species : Tetrahymena pyriformis (Protozoa)
Exposure period : 24 hour(s)
Unit : mg/l
EC50 : 160 -
Analytical monitoring : no data
Method : other: static at 30 degrees C
Year :
GLP : no data
Test substance : other TS: analytical grade

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
07.10.1994 (27)

Type :
Species : activated sludge
Exposure period : 3 hour(s)
Unit : mg/l
EC50 : 650 -
Method : OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year :
GLP :
Test substance :

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.08.1994 (23)

Type :
Species : activated sludge
Exposure period : 3 hour(s)
Unit : mg/l
EC50 : 650 -
Method : OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year :
GLP :
Test substance :

Source : Bayer AG Leverkusen
17.08.1994 (23)

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. Toxicity

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5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : 380 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 20
Vehicle : other: undiluted
Doses : 251, 316, 398 or 501 mg/kg bw
Method : other: Single Oral Dose, Younger Laboratories Protocol, 1976
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Four groups of male and female rats (5 animals/dose level) were fed a single oral dose of the undiluted test article via oral gavage. Male rats had initial body weights of 225-255 grams: females had initial body weights of 235-260 grams. Dosages were 251, 316, 398 and 501 mg/kg body weight.
Result : Clinical signs of toxicity included reduced activity and appetite (one to two days in survivors) followed by increasing weakness, collapse and death for decedents within several hours to two days, with most deaths occurring within one day. Gross autopsy findings on decedents were lung and liver hyperemia and gastrointestinal inflammation. Survivors were sacrificed after fourteen days. All viscera of survivors appeared normal.
LD50 = 380 mg/kg bw 95% confidence limits: 340-420 mg/kg.

Dose mg/kg	Mortalities		
	Male	Female	Combined
251	0/3	0/2	0/5
316	1/2	0/3	1/5
398	1/3	2/2	3/5
501	2/2	3/3	5/5

Test substance : purity: >96 %
Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag : Critical study for SIDS endpoint
18.06.2003

(28)

Type : LD50
Value : 492 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 20
Vehicle : other: Corn Oil (10% solution)
Doses : 398, 501, 631 or 794 mg/kg bw
Method : other: Oral LD50 by Single Oral Dose, Younger Laboratories Protocol, 1963
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Four groups of male and female rats (5 animals /dose level) were fed a single oral dose of the test article as a 10% solution in corn oil via stomach tube. Male rats had initial body weights of 225-265 grams: females had initial body weights of 210-240 grams. After the approximate Minimum Lethal Dose was determined, rats were fed in increasing doses at

5. Toxicity

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increments of 0.1 fractional log intervals at four levels designed to blanket the toxicity range. This supplied data for the calculation of the LD50, which was done according to a modification of the method of E.J. de Beer. Dosages were 398, 501, 631 and 794 mg/kg body weight. Observations were made for toxic signs and the viscera of the animals that died were examined macroscopically.

Result : Survival time was overnight to four days, with most deaths occurring in three to four days. Clinical signs of toxicity included tremors, diarrhea, increasing weakness, collapse and coma from 24 to 72 hours duration. At autopsy, findings of macroscopic examination were tissue edema, with liver and renal hyperemia.

<u>Dose mg/kg</u>	<u>Mortalities</u>		
	Male	Female	Combined
398	0/2	1/3	1/5
501	1/2	2/3	3/5
631	2/3	1/2	3/5
794	3/3	2/2	5/5

Test substance : purity: >96 %
Reliability : (2) valid with restrictions
age of study, lack of method detail

Flag : Critical study for SIDS endpoint

18.06.2003

(29)

Type : LD50
Value : = 479 - mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other
Year : 1986
GLP : yes
Test substance : other TS

Remark : value = 493.3 mg/kg (m), 465.6 mg/kg (f)
Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : purity: 99 %

27.07.1994

(30)

Type : LD50
Value : = 257 - mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other
Year : 1982
GLP : no
Test substance : no data

Remark : value = 0.206 ml/kg; density: 1.246 g/l; male rat
Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

27.07.1994

(31)

Type : LD50

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Value : = 177 - mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other
Year : 1982
GLP : no
Test substance : no data

Remark : value = 0.142 ml/kg; density: 1.246 g/l; female rat
Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
27.07.1994 (32)

Type : LD50
Value : -
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other
Year :
GLP : no data
Test substance : no data

Remark : dependent on the number of animals in each dose group LD50 values from 180 (1 rat/dose) to 375 mg/kg (5 rats/dose) were calculated
Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
27.07.1994 (33)

Type : LD50
Value : = 900 - mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other
Year :
GLP : no data
Test substance : no data

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
27.07.1994 (34)

Type : other
Value : -
Species : cat
Strain :
Sex :
Number of animals : 2
Vehicle : other: undiluted
Doses : 25 mg/kg bw

5. Toxicity

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Method : other
Year : 1985
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : 2 cats, 25 mg/kg with gavage: slightly elevated MetHb concentration (up to ca. 10 % after 3 hours), no effect after 7 hours; up to 100 % of the erythrocytes with Heinz bodies

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : purity: ca. 98 %
Reliability : (4) not assignable
18.06.2003 (35)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Value : ca. 5 - mg/l
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Exposure time : 4 hour(s)
Method : OECD Guide-line 403 "Acute Inhalation Toxicity"
Year : 1992
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : the following analytical concentrations were tested: 0.377 mg/l (vapour); 2.36 mg/l (aerosol) and 6.154 mg/l (aerosol) (analytical aerosol concentration)

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : purity: 97.4 %
Reliability : (1) valid without restriction
GLP Guideline study

Flag : Critical study for SIDS endpoint
16.06.2003 (36)

Type : LC50
Value : > 1400 - mg/m³
Species : rat
Strain : Sprague-Dawley
Sex : male
Number of animals : 4
Vehicle :
Doses :
Exposure time : 6 hour(s)
Method : other: A.T.S., 08/1973
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : Four male rats (weight 150 grams each) were placed in a glass dessicator, 250 mm diameter, and exposed for six hours to a concentrated atmosphere of vapors produced by passing a stream of air through 100ml of the test compound contained in a 250ml tall form gas washing bottle with fritted disc. Vapors from the bottle passed into a one liter bottle to remove droplets, and then on into the chamber. Air flow through the sample was 4

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liters/minute as measured by a calibrated rotameter. This air flow was sufficient to violently agitate the liquid. No supplementary air was introduced, as the above supply was ample for the animals' oxygen requirements. Air temperature was 77°F, and test chamber humidity was 54%. The volume of sample remaining after 6 hours was 98ml, indicating 2% vaporization.

Result : All animals survived the six hour exposure and the ten day observation period. Initial exposure produced signs of irritation (occasional pawing at nose, some ocular and nasal discharge during the first 5-10 minutes) and slight weakness. This improved after three to four hours, and at no time were the animals in danger of collapse. Breathing was nearly normal when the animals were removed from the test chamber. Inflammation of the nasal mucosa disappeared within two to three days. No respiratory complications were noted during the ten-day observation period.

Test substance : purity: >96%
Reliability : (1) valid without restriction
Guideline study
Flag : Critical study for SIDS endpoint

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(37)

Type : LC50
Value : -
Species : rat
Strain : Sprague-Dawley
Sex : male
Number of animals : 6
Vehicle :
Doses :
Exposure time : 6 hour(s)
Method : other: A.T.S., 08/1973
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Six male rats in a 35 liter (volume) test chamber were exposed to a stream of ambient air (air temperature 27°C, air flow rate of 4.0 l/min, chamber humidity of 80%) flowing over a reservoir containing 128.6 grams of the test material for 6 hours. At the conclusion of the test, the contents of the sample reservoir still weighed 128.6 grams, indicating that the test material was not volatile under test conditions.

Result : LC50 = Not determined - No vaporization of test material
The test animals exhibited no signs of toxicity. Following a 14-day observation period, all animals were sacrificed. All viscera appeared normal.

Test substance : purity: >96%

16.06.2003

(38)

Type : other: LC
Value : > 1.5 - mg/l
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Exposure time : 6 hour(s)
Method : other: no data
Year :
GLP : no data
Test substance : no data

Source : Bayer Antwerpen N.V. Antwerpen

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Reliability : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
: (4) not assignable
: data from secondary literature source
16.06.2003 (39)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : 933 - 1231 mg/kg bw
Species : rat
Strain :
Sex : male/female
Number of animals :
Vehicle : other: undiluted
Doses :
Method : other: Directive 84/449EEC, B.3.
Year : 1992
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : LD50: 1231 mg/kg (male), 933 mg/kg (female)
: NOEL = 500 mg/kg
Source : Bayer Antwerpen N.V. Antwerpen
: EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : purity: 97.4 %
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
18.06.2003 (40)

Type : LD50
Value : 400 - mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 20
Vehicle : other: undiluted
Doses : 316, 398, 501, 631 or 794 mg/kg bw
Method : other: Younger Laboratories Protocol B.1.30, Acute Dermal Toxicity by
: Single Dermal Application, 06/28/1984
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : The undiluted test substance was applied to the intact dorsal skin of male and female rabbits (2/sex/dose level) for a period of 24 hours, followed by a 14 day observation period. Initial weights for males in this study were 2.1-2.3 kg, and 2.2-2.3 kg for females. weighed. Dosages were 316, 398, 501, 631 or 794 mg/kg bw. Remaining test material was wiped from the exposed sites after 24 hours.

Result : LD50 = 500 mg/kg bw (males) C.I. = 355-700 mg/kg bw
: LD50 = 400 mg/kg bw (females) C.I. = 310-520 mg/kg bw
: LD50 = 400 mg/kg bw (combined) C.I. = 300-535 mg/kg bw

Clinical signs of toxicity included lethargy lasting up to two days, weakness and collapse. Deaths occurred in all but the lowest dose levels at 1-2 days after exposure. Necropsy findings included hemorrhagic areas of the lungs, liver, kidney and spleen discoloration, gall bladder enlargement and gastrointestinal inflammation. Surviving animals had no visible signs of pathology at necropsy, and all had gained weight.

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Dose mg/kg	Mortalities		
	Male	Female	Combined
316	0/2	0/2	0/4
398	1/2	1/2	2/4
501	1/2	2/2	3/4
631	1/2	2/2	3/4
794	2/2	2/2	4/4

Test substance : "Nitro composite" approximately 94%
Reliability : (1) valid without restriction
 Comparable to Guideline study
Flag : Critical study for SIDS endpoint

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(41)

Type : LD50
Value : 126 - 200 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 5
Vehicle : other: undiluted
Doses : 79.4, 126, 200, 398 or 501 mg/kg bw
Method : other: LD50 by Single Dermal Dose, Younger Laboratories Protocol, 1975
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : The undiluted test substance was applied to the shaved skin of male and female rabbits (1 animal/dose level) for a period of 24 hours, followed by a 14 day recovery period. Males in this study weighed 1.8-1.9 kg, and females weighed 1.9 kg. Dosages were 79.4, 126, 200, 398 or 501 mg/kg bw. The test material was held in place by means of an occlusive wrap of latex rubber and secured by bandaging and elastic tape. The occlusive wrap was removed after 24 hours and the excess material was wiped from the test animal.

Result : Clinical signs of toxicity were reduced appetite and activity -two to three days in survivors - followed by increasing weakness, collapse and death. Deaths occurred in 2-5 days. Gross autopsy findings on decedents included hemorrhagic areas of the lungs, liver, and spleen, kidney discoloration, enlarged gall bladder, and gastrointestinal inflammation. Survivors were sacrificed following the recovery period. All viscera appeared normal in these animals.

Dose mg/kg	Mortalities		
	Male	Female	Combined
79.4	0/1	---	0/1
126.0	---	0/1	0/1
200.0	1/1	---	1/1
398.0	---	1/1	1/1
501.0	1/1	---	1/1

Test substance : purity: 96%.
Reliability : (2) valid with restrictions
 age of study, lack of method detail

16.06.2003

(42)

Type : LDLo
Value : > 631 - mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 6
Vehicle : other: undiluted
Doses : 251, 398, 631, 1000, 1580 or 2510 mg/kg bw

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Method : other: Minimum Lethal Dose by Skin Absorption, Younger Laboratories Protocol, 1963
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : The undiluted test substance was applied in increasing doses at increments of 0.2 fractional log intervals to the closely clipped, intact skin of albino male and female rabbits. The treated areas were covered with plastic strips and the animals placed in wooden stocks for periods of up to 24 hours, after which time the test material was wiped away and the animals were placed into individual cages. Observations were made for toxic symptoms and the viscera of the animals that died on test were examined macroscopically.

Result : Clinical signs of toxicity were dyspnea, salivation, followed by weakness within two to four hours at the three highest dose levels. Survival times at the three highest doses were 8-24 hours. Animals given the three lower doses survived, and either gained or maintained weight. At autopsy, the only finding noted was pulmonary congestion.

Test substance : purity: 96%.
Reliability : (2) valid with restrictions
age of study, lack of method detail

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(43)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : LD50
Value : ca. 100 - 200 mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Route of admin. : i.p.
Exposure time :
Method : other: no data
Year :
GLP : no data
Test substance : no data

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

28.07.1994

(44)

Type : LD50
Value : = 95 - mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Route of admin. : i.v.
Exposure time :
Method : other: no data
Year :
GLP : no data
Test substance : no data

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

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28.07.1994 (45)

Type : LDLo
Value : -
Species : other
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Route of admin. : other
Exposure time :
Method : other: no data
Year :
GLP : no data
Test substance : no data

Remark : cat, i.v. 100 mg/kg; rat, i.v. 200-300 mg/kg;
rat, i.p. 1000 mg/kg; rat, oral 3000 mg/kg
Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

27.07.1994 (46)

Type : LD50
Value : = 310 - mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Route of admin. : other: no data
Exposure time :
Method : other: no data
Year :
GLP : no data
Test substance : no data

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

27.07.1994 (47)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 6
Vehicle :
PDII : .6
Result : slightly irritating
Classification : not irritating
Method : other: F.H.S.A./Draize, J.H., Woodard, G., and Calvery, H.O., 1944
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : 0.5ml of the undiluted test substance was applied to the shaved dorsal areas of six albino rabbits. The test material was applied to the skin under 1" square gauze patches and held in contact with the skin by means of an occlusive wrap of latex rubber secured by bandaging and elastic tape. The

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- occlusive wrap and gauze patches were removed after 24 hours. Dermal irritation was scored by the Draize Method, and results were recorded 24, 48, 72 and 168 hours after topical application. The Primary Irritation Index was calculated by averaging the mean scores at 24 and 72 hours and found to be 0.6 on a scale of 0.0-8.0.
- Result** : A slight defatting effect was noted - skin flaked off in seven to ten days. There was no injury in depth.
- Test substance** : purity: >96%
- Reliability** : (2) valid with restrictions
age of study, lack of method detail
- 18.06.2003 (48)
- Species** : rabbit
- Concentration** : undiluted
- Exposure** : Occlusive
- Exposure time** : 24 hour(s)
- Number of animals** : 3
- Vehicle** :
- PDII** : 3
- Result** : moderately irritating
- Classification** : irritating
- Method** : other: F.H.S.A./Draize, J.H., Woodard, G., and Calvery, H.O., 1944
- Year** :
- GLP** : no data
- Test substance** : as prescribed by 1.1 - 1.4
- Method** : The undiluted test substance was applied to the clipped, intact skin of three albino rabbits and removed after 24 hours. The application was covered with plastic strips to retard evaporation and avoid contamination. Observations were made at 1 hour, and then again at 24, 48, 72 and 120 hours. Dermal irritation was scored by the Draize Method.
- Result** : Redness developed within minutes. After one hour, there was a well-defined to moderate erythema with slight edema for an average score of 3.0 (out of 8.0) Edema disappeared in two animals in 24 hours, and inflammation reduced to slight redness in all animals within 72 hours. All animals scored "0" within 5 days.
- Test substance** : purity: >96%
- Reliability** : (2) valid with restrictions
age of study, lack of method detail, scoring at 1 hour instead of 24-72 hours
- 18.06.2003 (49)
- Species** : rabbit
- Concentration** :
- Exposure** :
- Exposure time** :
- Number of animals** :
- Vehicle** :
- PDII** :
- Result** : not irritating
- Classification** :
- Method** : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
- Year** : 1983
- GLP** : no
- Test substance** : no data
- Source** : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
- 18.06.2003 (50)

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5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : .1 ml
Exposure time : 24 hour(s)
Comment : not rinsed
Number of animals : 6
Vehicle :
Result : slightly irritating
Classification : not irritating
Method : other: F.H.S.A./Draize, J.H., Woodard, G., and Calvery, H.O., 1944
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : 0.1ml of the undiluted test compound was applied to one eye of six albino rabbits. The other eye was not treated and served as a control. The cornea, iris and conjunctiva were examined immediately after treatment, and then at intervals of 10 minutes, 1 hour, and then at 24, 48, 72, 120 and 168 hours. The Draize Method was used for scoring eye irritation.

Result : Exposure time Mean score (X/110)
1 hour 15.0
24 hours 23.5
48 hours 12.5
72 hours 4.8
120 hours 0.0
168 hours 0.0

Test substance : purity: 96%.

Reliability : (2) valid with restrictions
age of study, lack of method detail

18.06.2003

(51)

Species : rabbit
Concentration :
Dose :
Exposure time :
Comment :
Number of animals :
Vehicle :
Result : irritating
Classification :
Method : OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year : 1983
GLP : no
Test substance : no data

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

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(52)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic
Species : rat
Sex : male/female
Strain :
Route of admin. : oral feed
Exposure period : 6 months
Frequency of treatm. : daily

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Post exposure period : no data
Doses :
Control group : yes, concurrent vehicle
Method : other: no data
Year :
GLP : no
Test substance : no data

Remark : In a limited study, benzothiazole and similar compounds were administered to rats for six months in a dietary admixture. No evidence of carcinogenic activity was noted. No other data was presented.

Reliability : (3) invalid
Documentation insufficient for assessment

16.06.2003 (53)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Bacterial reverse mutation assay
System of testing : Salmonella typhimurium TA-98, TA-100, TA-1535, TA-1537, TA-1538
Test concentration : 0.001, 0.01, 0.10, 1.00 or 5.00 ul/plate (duplicate)
Cycotoxic concentr. : With and without metabolic activation: 5.00 ul/plate
Metabolic activation : with and without
Result : negative
Method : other: Ames Plate Test (Overlay method) 1975
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The Salmonella typhimurium strains used for this experiment were obtained from Dr. Bruce Ames. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. Chemicals used as positive controls for the non-activation assays were 10 ug/plate Methylnitrosoguanidine (MNNG), 100 ug/plate 2-nitrofluorene (NF) or 10 ug/plate Quinacrine mustard (QM). Positive controls used for the activation assays were 100 ug/plate 2-anthramine (ANTH), 100 ug/plate 2-Acetylaminofluorene (AAF) or 100 ug/plate 8-Aminoquinoline (AMQ). Dimethylsulfoxide (DMSO, 2.5%/plate) was used as the solvent and the solvent control. Statistical analysis was performed on plate incorporation assay results after transforming revertant/plate values as Log₁₀ (revertants/plate). Analysis included Bartlett's test for homogeneity of variance, and comparison of treatments with controls using within-levels pooled variance and a one-sided t-test. Grubbs' test was performed to determine if outliers were present.

Result : The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.
Positive control treatments produced the expected large increases in the frequency of histidine revertants.

Test substance : purity: >98%
Reliability : (1) valid without restriction
GLP Guideline study
Flag : Critical study for SIDS endpoint

16.06.2003 (54)

Type : Gene mutation in Saccharomyces cerevisiae
System of testing : Saccharomyces cerevisiae, D4
Test concentration : 0.001, 0.01, 0.10, 1.00 or 5.00 ul/plate (duplicate)

5. Toxicity

Id 95-16-9

Date 19.06.2003

Cycotoxic concentr. : With and without metabolic activation: 5.00 ul/plate
Metabolic activation : with and without
Result : negative
Method : other: Ames Mutagenicity Plate Test (Overlay Method) 1975
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : The test compound was evaluated for genetic activity with and without the addition of mammalian metabolic activation preparations. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. The chemical used as the positive control for the non-activation assay was methylnitrosoguanidine (MNNG) at 10 ug/plate. The positive control chemical used for the activation assay was DMNA at 100 micromoles/plate. Dimethylsulfoxide (DMSO, 2.5%/plate) was used as the solvent and the solvent control. Statistical analysis included Bartlett's test for homogeneity of variance, and comparison of treatments with controls using within-levels pooled variance and a one-sided t-test. Grubbs' test was performed to determine if outliers were present.

Result : The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.

Test substance : purity: >98%
Reliability : (1) valid without restriction
GLP Guideline study

18.06.2003

(54)

Type : Ames test
System of testing : S. typhimurium TA 98, TA 100, TA 1535, TA 1537
Test concentration : up to 5000 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other: see remark
Year : 1991
GLP : yes
Test substance : other TS

Remark : method: as described by Ames, B.N. et al., Proc. nat. Acad. Sci. (USA) 70, 2281-2285 (1973); Ames, B.N. et al., Mutat. Res. 31, 347-364 (1975) and Maron, D.M. & Ames, B.N., Mutat. Res. 113, 173-215 (1983)
No deviations from protocol noted.

Source : Bayer Antwerpen N.V. Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : purity: 97.4 %
Reliability : (1) valid without restriction
GLP Guideline study

18.06.2003

(55)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5. Toxicity

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5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

Endpoint	:	Neurotoxicity
Study descr. in chapter	:	
Reference	:	
Type	:	
Species	:	other: Cyprinodon variegates (Sheepshead Minnows)
Sex	:	
Strain	:	
Route of admin.	:	
No. of animals	:	
Vehicle	:	
Exposure period	:	
Frequency of treatm.	:	
Doses	:	3.75, 7.5, 15, 30 and 60 mg/l
Control group	:	
Observation period	:	
Result	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The neurotoxic potential of benzothiazole was investigated following in vivo and in vitro exposure of sheepshead minnows at the above doses. Following exposure, the test fish were evaluated for survival, growth and histological alterations
Remark	:	Benzothiazole cytotoxicity to primary cultures of brain cells from sheepshead minnow and tilapia (<i>Oreochromis niloticus</i>) and two epithelial cell lines was evaluated using a tetrazolium salt assay (MTT) at one and four days. The in vitro results indicated that primary cultures of brain cells are less sensitive to benzothiazole than epithelial cell lines. Significant cytotoxicity to the epithelial cell lines was noted at the two highest concentrations tested (30 mg/l and 60 mg/l).
Result	:	Fish mortality occurred after five days of exposure to the highest dose level of 60 mg/l. The LC50 value was determined to be 41.9 mg/l. Significant decreases in larval growth were noted at all test concentrations. Histologically, gills had cellular alterations but the central nervous system lacked severe cellular damage
Conclusion	:	Histologically and cytotoxicologically, the results indicated that benzothiazole is a gill toxicant but not a neurotoxicant.
Reliability	:	(4) not assignable Secondary literature
18.06.2003		(56)

5.10 EXPOSURE EXPERIENCE

Remark	:	Upon the flexor surface of the left wrist of 43 subjects (5f/38m) approx. 25 mg/kg were placed; 17 subjects with positive reactions (no further information)
Source	:	Bayer Antwerpen N.V. Antwerpen EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance	:	other TS
27.07.1994		(46)

6. Analyt. Meth. for Detection and Identification

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6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

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7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8. Meas. Nec. to Prot. Man, Animals, Environment

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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