

201-14881B1

I U C L I D

Data Set

RECEIVED
OPPT/CBIC
03 DEC -9 PM 12:29

Existing Chemical : ID: 102-60-3
CAS No. : 102-60-3
Common name : Quadrol
Molecular Formula : C14 H32 N2 O4
Molecular Weight : 292.42
Synonym : N,N,N',N'-tetrakis(2-hydroxypropyl)ethylenediamine

Producer related part
Company : Arcadis
Creation date : 20.09.2003

Substance related part
Company : Arcadis
Creation date : 20.09.2003

Status :
Memo :

Printing date : 01.12.2003
Revision date :
Date of last update : 01.12.2003

Number of pages : 13

Chapter (profile) : Chapter: 1.0.1, 1.1.0, 1.1.1, 1.2, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6.1, 3.1.1, 3.3.2, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.4, 5.5

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 102-60-3
Date 01.12.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : other
Name : Arcadis
Contact person : Jane Staveley
Date :
Street : 4915 Prospectus Drive, Suite F
Town : 27713 Durham, NC
Country : United States
Phone : 919-544-4535
Telefax :
Telex :
Cedex :
Email : jstaveley@arcadis-us.com
Homepage : www.arcadis-us.com

Remark : This document has been prepared on behalf of BASF Corporation
16.10.2003

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C14 H32 N2 O4
Molecular weight : 292.42
Petrol class :

29.09.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid
Purity : = 100 % w/w
Colour : white
Odour : mild polyol

02.10.2003 (1)

1.2 SYNONYMS AND TRADENAMES

1,1',1",1'''-(1,2-ethanediylidinitrilo)tetrakis-2-propanol
01.10.2003 (2)

2-propanol, 1,1',1",1'''-(1,2-ethanediylidinitrilo)tetrakis-
01.10.2003 (2)

Edetol
29.09.2003 (3)

1. General Information

Id 102-60-3
Date 01.12.2003

Entprol

01.10.2003 (2)

N,N,N',N'- tetrakis(2-hydroxypropyl)ethylenediamine

01.10.2003 (1)

Tetrahydroxypropyl Ethylenediamine

02.10.2003 (1)

2. Physico-Chemical Data

Id 102-60-3
Date 01.12.2003

2.1 MELTING POINT

Value : < 25 °C
Reliability : (2) valid with restrictions
Handbook data are assigned a reliability of 2
14.10.2003 (4)

2.2 BOILING POINT

Value : = 190 °C at 1.3332 hPa
01.10.2003 (2)

2.3 DENSITY

Type : relative density
Value : = 1.013 at °C
29.09.2003 (2)

2.4 VAPOUR PRESSURE

Value : = .000000012 hPa at °C
Decomposition :
Method : other (calculated): Modified Grain Method
Year :
GLP :
Test substance :
Method : MPBPWIN v1.41 (EPIWIN v3.11)
Remark : Calculated in mm Hg, converted to hPa
Reliability : (1) valid without restriction
calculated using scientifically acceptable method
14.10.2003

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log₁₀ K_{ow} : = -2.08 at °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance :
Method : KOWWIN v1.67 (EPIWIN v.3.11)
Reliability : (1) valid without restriction
calculated using scientifically acceptable method
13.10.2003

2. Physico-Chemical Data

Id 102-60-3
Date 01.12.2003

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ≥ 1000 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Remark : Quadrol is a base with pKa values of 4.30 and 8.99, respectively, for the two amine groups (McMahon, R., Brennan, M., and Glennon, J.D., Talanta 33(11):927 (1986).

Reliability : (2) valid with restrictions
Handbook data are assigned a reliability of 2

01.12.2003

(4)

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 : = .0000000002307401 cm³/(molecule*sec)
 Degradation : = 50 % after .6 hour(s)
 Deg. product :
 Method : other (calculated)
 Year :
 GLP :
 Test substance :

Method : AOPWIN v1.91 (EPIWIN v3.11)

Result :

AOP Program (v1.91) Results:

=====
 SMILES : OC(C)CN(CCN(CC(O)C)CC(O)C)CC(O)C
 CHEM : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediyldinitrilo)tetrakis-
 MOL FOR: C14 H32 N2 O4
 MOL WT : 292.42

----- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----

Hydrogen Abstraction = 98.1801 E-12 cm³/molecule-sec
 Reaction with N, S and -OH = 132.5600 E-12 cm³/molecule-sec
 Addition to Triple Bonds = 0.0000 E-12 cm³/molecule-sec
 Addition to Olefinic Bonds = 0.0000 E-12 cm³/molecule-sec
 Addition to Aromatic Rings = 0.0000 E-12 cm³/molecule-sec
 Addition to Fused Rings = 0.0000 E-12 cm³/molecule-sec

OVERALL OH Rate Constant = 230.7401 E-12 cm³/molecule-sec
 HALF-LIFE = 0.046 Days (12-hr day; 1.5E6 OH/cm³)
 HALF-LIFE = 0.556 Hrs

----- SUMMARY (AOP v1.91): OZONE REACTION -----

***** NO OZONE REACTION ESTIMATION *****
 (ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

Reliability : (1) valid without restriction
 calculated using scientifically acceptable method

14.10.2003

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
 Method : Calculation according Mackay, Level III
 Year :

Method : EPIWIN v3.11

Result :

Level III Fugacity Model (Full-Output):

=====

3. Environmental Fate and Pathways

Id 102-60-3

Date 01.12.2003

Chem Name : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediyldinitrilo)tetrakis-
Molecular Wt: 292.42
Henry's LC : 4.15e-016 atm-m3/mole (Henrywin program)
Vapor Press : 8.69e-009 mm Hg (Mpbpwin program)
Liquid VP : 1.62e-007 mm Hg (super-cooled)
Melting Pt : 154 deg C (Mpbpwin program)
Log Kow : -2.08 (Kowwin program)
Soil Koc : 0.00341 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	4.7e-008	1.11	1000
Water	49.8	900	1000
Soil	50.1	900	1000
Sediment	0.0918	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.42e-019	0.000693	1.11e-005	2.31e-005	3.71e-007
Water	8.37e-021	908	1.18e+003	30.3	39.3
Soil	3.11e-019	913	0	30.4	0
Sediment	7.71e-021	0.418	0.0435	0.0139	0.00145

Persistence Time: 789 hr
Reaction Time: 1.3e+003 hr
Advection Time: 2.01e+003 hr
Percent Reacted: 60.7
Percent Advected: 39.3

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 1.113
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.683 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Reliability : (1) valid without restriction
calculated using scientifically acceptable method
13.10.2003

3.5 BIODEGRADATION

Contact time :
Degradation : (±) % after
Result : other: not readily biodegradable
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance :
Method : BIOWIN v4.01 (EPIWIN v3.11)
Remark :

3. Environmental Fate and Pathways

Id 102-60-3
Date 01.12.2003

BIOWIN (v4.01) Program Results:

=====

SMILES : OC(C)CN(CCN(CC(O)C)CC(O)C)CC(O)C
CHEM : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediyldinitrilo)tetrakis-
MOL FOR: C14 H32 N2 O4
MOL WT : 292.42

----- BIOWIN v4.01 Results -----

Linear Model Prediction : Biodegrades Fast
Non-Linear Model Prediction: Does Not Biodegrade Fast
Ultimate Biodegradation Timeframe: Weeks-Months
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

Result
Reliability

: Summary output shown
: (1) valid without restriction
calculated using scientifically acceptable method

14.10.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
TLm	:	> 1000
TL1	:	> 1000
TL99	:	> 1000
Limit test	:	
Analytical monitoring	:	no
Method	:	
Year	:	1976
GLP	:	no
Test substance	:	
Method	:	Fathead minnows (35-50 mm length) were exposed to nominal concentrations of 0, 1.0, 10, 100 and 1000 ppm Quadrol using 10 fish per test concentration.
Result	:	No mortality was observed in any control or test concentration at any time during the study. No unusual behavioral reactions were noted among the exposed fish.
Test condition	:	Tests were conducted in reconstituted water with pH 7.2-7.6, hardness 40-48 ppm calcium carbonate, and alkalinity of 30-35 ppm calcium carbonate. Dissolved oxygen and pH was measured in the control every 24 hours and in all test concentrations and control at 96 hours. A reference toxicant test was performed on the same lot of fish using p,p-DDT.
Reliability	:	(2) valid with restrictions Study pre-dates standardized methods and GLP. Basic data provided but test conditions not completely described.

14.10.2003

(5)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	other: calculated
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 1435 calculated
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Method	:	ECOSAR v0.99g (EPWIN v3.11)
Result	:	Class: aliphatic amines
Reliability	:	(1) valid without restriction calculated using scientifically acceptable method

14.10.2003

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: green algae
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l

4. Ecotoxicity

Id 102-60-3
Date 01.12.2003

EC50 : = 662 calculated
Method : other: calculated
Year :
GLP :
Test substance :

Method : ECOSAR v0.99g (EPIWIN v3.11)
Result : Class: aliphatic amines
Reliability : (1) valid without restriction
calculated using scientifically acceptable method

14.10.2003

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 11200 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	male
Number of animals	:	10
Vehicle	:	water
Doses	:	4400, 5600, 7500, 9750, 12600, 16500 mg Quadrol/kg
Method	:	other: study pre-dates standardized methods
Year	:	1956
GLP	:	no
Test substance	:	
Method	:	Doses prepared as 20% solution of Quadrol in water, neutralized to pH 7. Administered by stomach tube to male albino rats weighing approximately 100 grams. Animals observed for approximately one week following administration.
Reliability	:	(2) valid with restrictions Study pre-dates GLPs and standardized methods. Basic documentation provided, details of methods lacking

14.10.2003

(6)

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-acute
Species	:	rat
Sex	:	male/female
Strain	:	other: Harlan albino
Route of admin.	:	oral feed
Exposure period	:	three months
Frequency of treatm.	:	ad libitum
Post exposure period	:	no post-exposure observation period
Doses	:	Doses were equivalent to average daily intakes of 70, 210, 720, 2170 and 3750 mg/kg bw
Control group	:	yes, concurrent no treatment
NOAEL	:	ca. 600 - 900 mg/kg
Method	:	
Year	:	1956
GLP	:	no
Test substance	:	
Method	:	10 males and 10 females were used in each group (5 doses and untreated control). Doses were administered as 0.1%, 0.3%, 1%, 3% and 5% Quadrol in the feed. Body weight and feed consumption were determined weekly. Hematology parameters (hemoglobin concentration, erythrocyte counts, total white cell counts, and differential white cell counts) were determined at the initiation and termination of exposure. At termination, prothrombin time and organ weights (lungs, liver, spleen, kidneys, adrenal glands, gonads and pancreas), as well as liver fat, were determined.
Result	:	Animals in the two highest dose groups exhibited temporary decreased food consumption, loss of body weight, and interference with growth rate. After the first month, however, food intake and rate of growth was similar in all groups. Rats fed Quadrol at levels up to 1% of the diet (representing a dosage of 600 - 900 mg/kg/d) exhibited no signs of toxicity. Rats fed Quadrol at levels of 3% and 5% of the diet (reaching a maximum daily dose

of 3300 mg/kg in the first week) suffered some failure to gain weight in the early weeks of the experiment, possibly due to unpalatability of the diet. In these higher dose groups no other evidence of toxicity was seen, except for a slightly greater incidence of borderline abnormalities of the liver, which were of questionable significance.

Reliability : (2) valid with restrictions
Study pre-dates GLPs and standardized methods. Basic documentation provided, details of methods lacking.

14.10.2003 (7)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium TA97, TA98, TA100, TA 102; E. coli WP2(PKM101)
Test concentration : 200 - 10000 ug/plate (test material solvent: DMSO)
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other: only referred to as "standard plate"
Year : 1994
GLP : no data
Test substance : no data

Reliability : (4) not assignable
secondary reference (from CCRIS in TOXNET)

14.10.2003 (8)

9. References

Id 102-60-3
Date 01.12.2003

- (1) MSDS, BASF Corp., 17 SEP 2002
- (2) MSDS, MDL Information Systems, 11 DEC 2001
- (3) MSDS, MDL Information Systems, 22 MAR 2001
- (4) Budavari, S., ed., The Merck Index: an encyclopedia of chemicals, drugs and biologicals. 12th ed., Merck and Co., New Jersey, 1996.
- (5) Industrial Bio-Test Laboratories, Report No. 8560-08828, Four-Day Static Aquatic Toxicity Study with Quadrol in Fathead Minnows, May 4, 1976.
- (6) Hill Top Research Institute, Acute Oral Toxicity of Quadrol, March 7, 1956
- (7) Hill Top Research Institute, Subacute Oral Toxicity of Quadrol, March 1, 1956, Project 151.
- (8) Hachiya, N. and Takizawa, Y., Mutagenicity of Plastic Additives, Hen'igensei Shiken 3(3):147-154 (1994). Cited at <http://toxnet.nlm.nih.gov>, CCRIS Record number 8275, last updated 02/12/2001.

I U C L I D

Data Set

RECEIVED
OPPT/CBIC
03 DEC -9 PM 12: 29

Existing Chemical : ID: 122-20-3
 CAS No. : 122-20-3
 EINECS Name : 1,1',1"-nitrilotripropan-2-ol
 Common Name : triisopropanolamine
 EC No. : 204-528-4
 TSCA Name : 2-Propanol, 1,1',1"-nitrilotris-
 Molecular Formula : C9H21NO3

Producer related part
 Company : Arcadis
 Creation date : 02.10.2003

Substance related part
 Company : Arcadis
 Creation date : 02.10.2003

Status :
 Memo :

Printing date : 01.12.2003
 Revision date :
 Date of last update : 01.12.2003

Number of pages : 16

Chapter (profile) : Chapter: 1.0.1, 1.1.0, 1.1.1, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6.1, 2.7, 2.14, 3.1.1,
 3.3.2, 3.5, 3.6, 4.1, 4.2, 4.3, 4.4, 4.9, 5.1.1, 5.4, 5.5, 5.6, 5.8.1, 5.8.2, 5.8.3

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 122-20-3
Date 01.12.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : other
Name : Arcadis
Contact person : Jane Staveley
Date :
Street : 4915 Prospectus Drive, Suite F
Town : 27713 Durham, NC
Country : United States
Phone : 919-544-4535
Telefax : 919-544-5690
Telex :
Cedex :
Email : jstaveley@arcadis-us.com
Homepage : www.arcadis-us.com

Remark : This document has been prepared on behalf of BASF Corporation

15.10.2003

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C9 H21 NO3
Molecular weight : 191.27
Petrol class :

07.10.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status :
Purity : >= 97 % w/w
Colour :
Odour :

Method : GC

02.10.2003

(1)

2.1 MELTING POINT

Value : ca. 50 °C

Source : BASF AG Ludwigshafen
02.12.1992

(2)

2.2 BOILING POINT

Value : = 134.2 °C at 1.25 hPa
Decomposition :
Method : other: vapour pressure measurement
Year : 1972
GLP : no
Test substance :

Method : Dynamic method
Result : measured values:

temperature (°C)	vapour pressure (torr)	vapour pressure (hPa)
134.2	0.94	1.25
144.7	1.74	2.31
155.7	3.18	4.24
165.3	5.30	7.07
175.9	8.88	11.84
186.2	14.3	19.07
198.8	24.9	33.20
199.8	25.5	34.00
214.4	45.3	60.40
228.3	80.1	106.80
244.8	140.0	186.65
263.6	240.0	319.97
267.5	320.2	426.90
270.4	338.1	450.76
272.6	329.8	439.70
277.0	355.5	473.96
287.5	530.0	706.61
301.1	760.0	1013.25

The regression of the results leads with a mean deviation of 3.18 % to the following equation:

$$P.VL(T) = EXP(A + B/T + C*LN(T) + D*T**E)$$

A = 838.1367
 B = -42064.89
 C = -130.1468
 D = 0.1279836
 E = 1

Source : BASF AG Ludwigshafen
Test substance : Triisopropanolamine, no further data
Reliability : (2) valid with restrictions
 Acceptable study, meets basic scientific principles

22.10.2003

(3)

2.3 DENSITY

Type : density
 Value : = 1.01 g/cm³ at 60 °C
 Remark : DIN 51757
 Source : BASF AG Ludwigshafen
 02.12.1992

(2)

2.4 VAPOUR PRESSURE

Value : = .000000018084 hPa at 25 °C
 Decomposition :
 Method : other (measured)
 Year : 1972
 GLP : no
 Test substance :

Method : Dynamic method
 Result : measured values:

temperature (°C)	vapour pressure (torr)	vapour pressure (hPa)
134.2	0.94	1.25
144.7	1.74	2.31
155.7	3.18	4.24
165.3	5.30	7.07
175.9	8.88	11.84
186.2	14.3	19.07
198.8	24.9	33.20
199.8	25.5	34.00
214.4	45.3	60.40
228.3	80.1	106.80
244.8	140.0	186.65
263.6	240.0	319.97
267.5	320.2	426.90
270.4	338.1	450.76
272.6	329.8	439.70
277.0	355.5	473.96
287.5	530.0	706.61
301.1	760.0	1013.25

The regression of the results leads with a mean deviation of 3.18 % to the following equation:

$$P.VL(T) = \text{EXP}(A + B/T + C \cdot \text{LN}(T) + D \cdot T^{**}E)$$

A = 838.1367
 B = -42064.89
 C = -130.1468
 D = 0.1279836
 E = 1

The Vapour Pressure at 20 °C, 25 °C and 50 °C was calculated from the regression equation:

temperature (°C)	vapour pressure (hPa)
20	7.7665E-09
25	1.8084E-08

2. Physico-Chemical Data

Id 122-20-3
Date 01.12.2003

Source : 50 6.8550E-07
Test substance : BASF AG Ludwigshafen
Reliability : Triisopropanolamine, no further data
(2) valid with restrictions
Acceptable study, meets basic scientific principles
22.10.2003 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log p_{ow} : = -.015 at °C
pH value :
Method : OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year : 1987
GLP :
Test substance :
Source : BASF AG Ludwigshafen
16.10.2003 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : > 1000 g/l at 20 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : 7.86 at 25 °C
Description :
Stable :
01.12.2003 (5) (6)

2.7 FLASH POINT

Value : = 160 °C
Type : closed cup
Method : other: DIN 51758
Year :
GLP :
Test substance :
Source : BASF AG Ludwigshafen
02.12.1992 (2)

2.14 ADDITIONAL REMARKS

Remark : Explosionsgrenzen in Luft: 0.8 - 5.8 Vol. %
Zuendtemperatur: 275 Grad C (DIN 51794)
Gefahrliche Reaktionen: exotherme Reaktion mit Saeuren
Source : BASF AG Ludwigshafen
02.12.1992 (2)

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 : = .00000000124029 cm³/(molecule*sec)
Degradation : 50 % after .1 day(s)

Method : APOWIN v1.91 (EPIWIN v3.11)
Remark : assumed data: 1.5E6 OH/cm³; 12-h day
Result :

AOP Program (v1.91) Results:
 =====
 SMILES : OC(C)CN(CC(O)C)CC(O)C
 CHEM : 2-Propanol, 1,1',1"-nitrilotris-
 MOL FOR: C9 H21 N1 O3
 MOL WT : 191.27
 ----- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----
 Hydrogen Abstraction = 57.6090 E-12 cm³/molecule-sec
 Reaction with N, S and -OH = 66.4200 E-12 cm³/molecule-sec
 Addition to Triple Bonds = 0.0000 E-12 cm³/molecule-sec
 Addition to Olefinic Bonds = 0.0000 E-12 cm³/molecule-sec
 Addition to Aromatic Rings = 0.0000 E-12 cm³/molecule-sec
 Addition to Fused Rings = 0.0000 E-12 cm³/molecule-sec

 OVERALL OH Rate Constant = 124.0290 E-12 cm³/molecule-sec
 HALF-LIFE = 0.086 Days (12-hr day; 1.5E6 OH/cm³)
 HALF-LIFE = 1.035 Hrs
 ----- SUMMARY (AOP v1.91): OZONE REACTION -----

 ***** NO OZONE REACTION ESTIMATION *****
 (ONLY Olefins and Acetylenes are Estimated)

Reliability : Experimental Database: NO Structure Matches
 : (1) valid without restriction
 : calculated using scientifically acceptable method
 15.10.2003

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Method : EPIWIN v3.11
Result :

Level III Fugacity Model (Full-Output):
 =====
 Chem Name : 2-Propanol, 1,1',1"-nitrilotris-
 Molecular Wt: 191.27
 Henry's LC : 9.77e-012 atm-m³/mole (Henrywin program)
 Vapor Press : 1.86e-005 mm Hg (Mpbpwin program)
 Liquid VP : 6.31e-005 mm Hg (super-cooled)
 Melting Pt : 78.6 deg C (Mpbpwin program)

3. Environmental Fate and Pathways

Id 122-20-3

Date 01.12.2003

Log Kow : -1.22 (Kowwin program)
Soil Koc : 0.0247 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000321	2.07	1000
Water	45.3	360	1000
Soil	54.6	360	1000
Sediment	0.0755	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	5.1e-015	1.36	0.0405	0.0452	0.00135
Water	1.46e-016	1.1e+003	572	36.7	19.1
Soil	6.5e-015	1.33e+003	0	44.2	0
Sediment	1.22e-016	0.459	0.0191	0.0153	0.000635

Persistence Time: 420 hr
Reaction Time: 519 hr
Advection Time: 2.21e+003 hr
Percent Reacted: 80.9
Percent Advected: 19.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 2.07
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 3.002 (weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Reliability : (1) valid without restriction
calculated using scientifically acceptable method
16.10.2003

3.5 BIODEGRADATION

Type :
Inoculum : activated sludge, industrial
Concentration : 400 mg/l related to
related to
Contact time :
Degradation : < 10 (±) % after 28 day(s)
Result : other: poorly eliminated from water
Deg. product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens
Test"
Year :
GLP : no
Test substance :
Remark : Other information (Davis and Carpenter, 1997) indicates that
biodegradation of triisopropanolamine increases from a 5-day BOD value
of <5% using an unacclimated inoculum to 40-50% using an acclimated

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inoculum. In a simulation test with dilute activated sludge, diisopropanolamine was completely degraded within 72-120 hours; since this compound is a major metabolite of the aerobic biodegradation of triisopropanolamine, similar results would be expected for triisopropanolamine (Davis, J.W. and Carpenter, C.L., 1997. Environmental assessment of the alkanolamines. Reviews of Environmental Contamination and Toxicology, Vol. 149, pp. 87-137).

Source
24.11.2003

: BASF AG Ludwigshafen

(7)

3.6 BOD5, COD OR BOD5/COD RATIO

Method

: DIN 38409 T51
DIN 38409 T41

Remark

: inoculum:
effluent of an industrial waste water treatment plant

Result

: COD: 1963 mg/g
BOD5: <2 mg/g
TOC: 556 mg/g
BOD5*100/COD: 0 % (no degradation)

Source

: BASF AG Ludwigshafen

Reliability

: (2) valid with restrictions
test according to National Standard with restriction

03.09.2003

(8)

4. Ecotoxicity

Id 122-20-3
Date 01.12.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Leuciscus idus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : > 2150 - 4640
Limit test :
Analytical monitoring : no
Method : other: German Industrial Standard DIN 38412, Part 15
Year : 1987
GLP : no
Test substance : other TS: triisopropanolamine, purity: >99 %

Method : Test concentrations of 1000, 2150, 4650 and 10000 mg/L were prepared in reconstituted fresh water, hardness 2.5 mmol/L, pH approx. 8.0.
Result : The 96-h LC50 was between 2200 and 4600 mg/L, with no effects at the former value and 100% mortality at the latter value.
Source : BASF AG Ludwigshafen
Reliability : (1) valid without restriction
Test conducted according to standard procedure and with appropriate documentation.

15.10.2003

(9)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : other aquatic arthropod: Daphnia magna Straus
Exposure period : 48 hour(s)
Unit : mg/l
EC0 : = 250
EC50 : > 500
EC100 : > 500
Analytical monitoring : no
Method : other: Directive 79/831/EEC, Annex V, Part C
Year : 1988
GLP : no
Test substance : other TS: triisopropanolamine

Result : effect values after 24 h (related to nominal concentrations):
EC0 (24 h): =250 mg/L
EC50 (24 h): >500 mg/L
EC100 (24 h): >500 mg/L
Source : BASF AG Ludwigshafen
Reliability : (1) valid without restriction
Test conducted according to standard procedure and with appropriate documentation.

15.10.2003

(10)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Scenedesmus subspicatus (Algae)
Endpoint : biomass
Exposure period : 72 hour(s)
Unit : mg/l
EC10 : = 8.84

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EC50 : = 68.93
EC90 : > 100
Limit test :
Analytical monitoring : no
Method : other: German Industrial Standard DIN 38412, Part 9
Year :
GLP : no
Test substance : other TS: triisopropanolamine, purity: >98 %

Remark : Effect values were originally reported based upon inhibition of fluorescence at 72 h. These results were:
EC20 = 11 mg/L
EC50 = 35 mg/L
EC90 > 100 mg/L

Effect values were recalculated according to OECD Guideline 201 for growth rate and biomass using linear regression analysis considering fluorescence values mentioned in the report (BASF AG, Department of Ecology, unpublished data, 1090/88, 19.12.1990). This recalculation yielded 72 h growth rate values of:

ErC10 = 16.1 mg/L
ErC50 > 100 mg/L
ErC90 > 100 mg/L

and biomass values of:
EbC10 = 8.84 mg/L
EbC50 = 68.93 mg/L
EbC90 > 100.0 mg/L

Result : The most sensitive results are those based upon biomass.
effect values related to nominal concentration of the test substance.

Source : BASF AG Ludwigshafen
Reliability : (1) valid without restriction
test procedure according to National Standard (German Industrial Standard DIN)

15.10.2003 (11) (12)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic
Species : activated sludge, industrial
Exposure period : 30 minute(s)
Unit : mg/l
EC20 : > 1995
Analytical monitoring : no
Method : other
Year :
GLP : no
Test substance :

Remark : Bei sachgemaesser Einleitung in adaptierte biologische Klaer- anlagen sind keine Stoerungen der Abbauaktivitaet des Belebt- schlammms zu erwarten.
Hoechste getestete Konzentration: 1995 mg/l; foerdernde Wirkung.

Source : BASF AG Ludwigshafen
03.09.2003 (7)

4. Ecotoxicity

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Type : aquatic
Species : Pseudomonas putida (Bacteria)
Exposure period : 18 hour(s)
Unit : mg/l
TGK : = 20000
Analytical monitoring : no
Method : other: following DIN 38 412, Part 8
Year :
GLP : no
Test substance :

Method : test substance tested after neutralization
Source : BASF AG Ludwigshafen
Reliability : (4) not assignable
original reference not available

03.09.2003 (13)

4.9 ADDITIONAL REMARKS

Memo : Further information can be taken from the BUA report No. 148 (Triisopropanolamin).

Source : BASF AG Ludwigshafen
22.12.1999

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : = 6500 mg/kg bw
Species : rat
Strain : Wistar
Sex : male
Number of animals : 10
Vehicle : water
Doses : Minimum: 140 mg/kg. Maximum: 1350 mg/kg.
Method : other
Year : 1941
GLP : no
Test substance :

Method : Animals were dosed via gastric tube to the test substance diluted in water.
Remark : The results of this study are supported by other reported oral LD50 values for the rat ranging from 4000 to 9000 mg/kg bw (BUA Report 148, Triisopropanolamine, German Chemical Society Advisory Committee on Existing Chemicals of Environmental Relevance, December, 1993).
Result : The maximum dose having no effect was 140 mg/kg bw.
Reliability : (2) valid with restrictions
 Study pre-dates standardized methods and GLP. Test conditions not fully described.

22.10.2003

(14)

5.4 REPEATED DOSE TOXICITY

Type :
Species : rat
Sex : male
Strain : Wistar
Route of admin. : oral feed
Exposure period : 102 weeks
Frequency of treatm. :
Post exposure period :
Doses : Single dose, approximately equal to 1216 mg/kg bw/day
Control group : yes, concurrent no treatment
NOAEL : > 1216 mg/kg bw
Method : other
Year : 1991
GLP : no data
Test substance :

Method : The 2% dose was reported as equal to 324 mg/day per animal. Based upon the reported average initial and final body weights, this dose was calculated to be approximately equal to 1216 mg/kg bw/day

Result : This study, designed to examine carcinogenic effects, used a single group of 19 rats exposed to 2% triisopropanolamine and 17 controls. None of 19 exposed rats demonstrated tumors in the nasal cavity, lung, esophagus, liver, urinary bladder, thyroid, kidney, stomach, pancreas, or mammary gland. Pheochromocytoma (adrenal gland) and Leydig cell tumors (testis) were observed but at similar or lower percentages than observed in the controls. There was a 5% incidence (1 animal of 19) of pituitary gland adenomas in the treated rats versus none in the controls and an 11% incidence (2 animals of 19) of "other" tumors versus 18% in the controls; neither of these effects was statistically significant.

Test condition : Test conditions not described in English

5. Toxicity

Id 122-20-3

Date 01.12.2003

Reliability	:	(4) not assignable Insufficient documentation	
22.10.2003			(15)
Type	:		
Species	:	rat	
Sex	:	male/female	
Strain	:	no data	
Route of admin.	:	drinking water	
Exposure period	:	30 days	
Frequency of treatm.	:	continuously in the drinking water	
Post exposure period	:	no data	
Doses	:	140 mg/kg - 1350 mg/kg	
Control group	:	yes, concurrent no treatment	
NOAEL	:	140 mg/kg	
Method	:	other	
Year	:		
GLP	:	no	
Test substance	:		
Method	:	Animals (5 per dose) were exposed to triisopropanolamine in the drinking water for 30 days.	
Result	:	The highest dose level reduced food intake and growth. 260 mg/kg still caused micropathological lesions of liver, kidney, spleen or testes (scope of examinations or kind of lesions are not mentioned). No treatment-related deaths occurred during the study.	
Reliability	:	(2) valid with restrictions Study pre-dates standardized methods and GLP. Test conditions not fully described.	
01.12.2003			(16)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test	
System of testing	:	Salmonella typhimurium TA98, TA100, TA1535, TA1537	
Test concentration	:	up to 10 mg/plate	
Cycotoxic concentr.	:		
Metabolic activation	:	with and without	
Result	:	negative	
Method	:	other: according to Haworth, S. et al.: Environ. Mutagen. 5, Suppl. 1, 3-142	
Year	:	1983	
GLP	:	no data	
Test substance	:	as prescribed by 1.1 - 1.4	
Source	:	BASF AG Ludwigshafen	
05.12.1993			(17)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Micronucleus assay	
Species	:	mouse	
Sex	:	male/female	
Strain	:	NMRI	
Route of admin.	:	gavage	
Exposure period	:		
Doses	:	500, 1000, 2000 mg/kg bw in a volume of 10ml/kg bw	
Result	:		

5. Toxicity

Id 122-20-3

Date 01.12.2003

Method : OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year :
GLP : yes
Test substance : other TS

Remark : According to the results of the present study, the single oral administration of Triisopropanolamin did not lead to any increase in the number of polychromatic erythrocytes containing either small or large micronuclei.
No inhibition of erythropoiesis determined from the ratio of polychromatic to normochromatic erythrocytes was detected.
Triisopropanolamin does not have any chromosome-damaging effect, and there were no indications of any impairment of chromosome distribution in the course of mitosis.

Source : BASF AG Ludwigshafen
Test substance : degree of purity: 92.0%
21.06.1996

(18)

5.8.1 TOXICITY TO FERTILITY

Type : other: no data
Species : rat
Sex : female
Strain : no data
Route of admin. : other: no data (presumably orally)
Exposure period : throughout pregnancy (no further data)
Frequency of treatm. : no data
Premating exposure period
 Male :
 Female :
Duration of test : no data
No. of generation :
studies
Doses : 0.063 mg/kg/d
Control group : no data specified
Method : other: no data
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : no malformations, no adverse effects on reproductive parameters; original source not available

Source : BASF AG Ludwigshafen
05.12.1993

(19)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Wistar
Route of admin. : gavage
Exposure period : on day 6 through day 15 p.c.
Frequency of treatm. : daily
Duration of test : until day 20 p.c.
Doses : 100; 400; 1000 mg/kg
Control group : yes
NOAEL maternal tox. : 400 mg/kg bw

5. Toxicity

Id 122-20-3

Date 01.12.2003

NOAEL teratogen.	:	>= 1000 mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	
GLP	:	yes
Test substance	:	other TS
Result	:	The test substance was administered as an aqueous solution to 23-25 pregnant rats/group. In the 1000 mg/kg dose group statistically significantly decreased food consumption at the beginning of the treatment period and significantly reduced body weight gain were observed. There were no effects on gestational parameters or fetuses. No substance-related effects on dams or fetuses were found in the other groups.
Source	:	BASF AG Ludwigshafen
Test substance	:	Triisopropanolamine, purity 92 %
22.10.2003		

(20)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type	:	
In vitro/in vivo	:	In vivo
Species	:	rat
Sex	:	male
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	102 weeks
Frequency of treatm.	:	
Duration of test	:	102 weeks
Doses	:	Single dose, approximately equal to 1216 mg/kg bw/day
Control group	:	yes, concurrent no treatment
Method	:	other: study was designed to examine carcinogenic effects
Year	:	1991
GLP	:	no data
Test substance	:	
Method	:	The 2% dose was reported as equal to 324 mg/day per animal. Based upon the reported average initial and final body weights, this dose was calculated to be approximately equal to 1216 mg/kg bw/day.
Result	:	This study, designed to examine carcinogenic effects, used a single group of 19 rats exposed to 2% triisopropanolamine and 17 controls. None of 19 exposed rats demonstrated a significant increase in tumors of reproductive organs relative to the controls. This included the testis, mammary gland and pituitary gland.
Test condition	:	Test conditions not described in English
Reliability	:	(4) not assignable Insufficient documentation
16.10.2003		

(15)

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