

201-15441B1

# I U C L I D

## Data Set

RECEIVED  
OPT. CHIC  
2004 JUL 12 PM 12:06

**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** : 29.06.2004  
**Revision date** :  
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**Number of pages** : 14

**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, 3.1.2, 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 29.06.2004

## 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 :  
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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 29.06.2004

### 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 29.06.2004

### 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  
**Decomposition** :  
**Method** : other  
**Year** :  
**GLP** :  
**Test substance** :  
**Method** : It is not known whether the value was measured or calculated.  
21.06.2004 (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  
**Log *p*<sub>ow</sub>** : = -2.08 at °C  
**pH value** :  
**Method** : other (calculated)  
**Year** :  
**GLP** :  
**Test substance** :  
**Method** : KOWWIN v1.67 (EPIWIN v.3.11)

## 2. Physico-Chemical Data

Id 102-60-3

Date 29.06.2004

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

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

**Solubility in** : Water  
**Value** :  $\geq 1000$  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. Environmental Fate and Pathways

Id 102-60-3  
Date 29.06.2004

#### 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 cm<sup>3</sup>/(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 cm<sup>3</sup>/molecule-sec  
Reaction with N, S and -OH = 132.5600 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Triple Bonds = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Olefinic Bonds = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Aromatic Rings = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Fused Rings = 0.0000 E-12 cm<sup>3</sup>/molecule-sec

OVERALL OH Rate Constant = 230.7401 E-12 cm<sup>3</sup>/molecule-sec  
HALF-LIFE = 0.046 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)  
HALF-LIFE = 0.556 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  
14.10.2003

#### 3.1.2 STABILITY IN WATER

Type : abiotic  
t1/2 pH4 : at °C  
t1/2 pH7 : at °C  
t1/2 pH9 : at °C

Remark : Due to the lack of hydrolyzable functional groups, Quadrol is expected to  
be stable to hydrolysis.  
21.06.2004

### 3. Environmental Fate and Pathways

Id 102-60-3  
Date 29.06.2004

#### 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'',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

### 3. Environmental Fate and Pathways

Id 102-60-3

Date 29.06.2004

**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** :

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

14.10.2003

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

<b>Type</b>	:	static
<b>Species</b>	:	Pimephales promelas (Fish, fresh water)
<b>Exposure period</b>	:	96 hour(s)
<b>Unit</b>	:	mg/l
<b>TLm</b>	:	> 1000
<b>TL1</b>	:	> 1000
<b>TL99</b>	:	> 1000
<b>Limit test</b>	:	
<b>Analytical monitoring</b>	:	no
<b>Method</b>	:	
<b>Year</b>	:	1976
<b>GLP</b>	:	no
<b>Test substance</b>	:	other TS
<b>Method</b>	:	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.
<b>Result</b>	:	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. Dissolved oxygen levels at 96 hours ranged from 5.2 mg/L in the 100 ppm test concentration to 6.4 mg/L in the control, while pH at 96 hours ranged from 7.2 in the control to 9.2 in the highest test concentration. The Litchfield-Wilcoxon method was used to calculate the TL-50.
<b>Test condition</b>	:	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. The test temperature was not reported; however, it was stated that the fish were held at 18 degrees prior to testing. 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.
<b>Test substance</b>	:	Test substance identified as Quadrol, but no information given about purity.
<b>Reliability</b>	:	(2) valid with restrictions Study pre-dates standardized methods and GLP. Basic data provided but test conditions not completely described.

21.06.2004

(5)

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

<b>Type</b>	:	other: calculated
<b>Species</b>	:	Daphnia sp. (Crustacea)
<b>Exposure period</b>	:	48 hour(s)
<b>Unit</b>	:	mg/l
<b>EC50</b>	:	= 1435 calculated
<b>Method</b>	:	other: calculated
<b>Year</b>	:	
<b>GLP</b>	:	
<b>Test substance</b>	:	
<b>Method</b>	:	This estimate of the toxicity of Quadrol was made using ECOSAR v0.99g (EPWIN v3.11) using the SAR equation for the aliphatic amines class. The only input information was the CAS No. The octanol water partition coefficient was calculated using CLOGP, Ver. 3.3. The SAR equation used was $\text{Log } 48\text{-h LC}_{50} \text{ (millimoles/L)} = -0.524 - 0.584 \log Kow$ , where $N=10$ , $R^2=0.78$ , $\log Kow < 5.0$ , $MW < 1000$
<b>Result</b>	:	ECOSAR Program (v0.99g) Results:

## 4. Ecotoxicity

Id 102-60-3

Date 29.06.2004

=====  
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-  
CAS Num: 000102-60-3  
ChemID1:  
ChemID2:  
ChemID3:  
MOL FOR: C14 H32 N2 O4  
MOL WT : 292.42  
Log Kow: -2.08 (KowWin estimate)  
Melt Pt:  
Wat Sol: 1.886E+007 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

-----  
Aliphatic Amines

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	1.41e+006
Aliphatic Amines	: Fish	96-hr	LC50	32901.113
Aliphatic Amines	: Daphnid	48-hr	LC50	1434.599
Aliphatic Amines	: Green Algae	96-hr	EC50	661.806
Aliphatic Amines	: Green Algae	96-hr	ChV	57.774

Note: \* = asterick designates: Chemical may not be soluble enough to measure this predicted effect.  
Fish and daphnid acute toxicity log Kow cutoff: none  
Green algal EC50 toxicity log Kow cutoff: none  
Chronic toxicity log Kow cutoff: none  
MW cutoff: none

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

21.06.2004

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** : other algae: green algae  
**Endpoint** :  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**EC50** : = 662 calculated  
**ChV** : = 57.7 calculated  
**Method** : other: calculated  
**Year** :  
**GLP** :  
**Test substance** :

**Method** : This estimate of the toxicity of Quadrol was made using ECOSAR v0.99g (EPIWIN v3.11) using the SAR estimation for the aliphatic amine class. The only input information was the CAS No. The octanol water partition coefficient was calculated using CLOGP, Ver. 3.3. The SAR equation used to estimate the ChV was:  $\text{Log ChV (millimoles/L)} = -1.399 - 0.334 \log\text{Kow}$ ,

## 4. Ecotoxicity

Id 102-60-3

Date 29.06.2004

### Result

where N=11, R<sup>2</sup>=0.61, logKow<7.0, MW<1000. The SAR equation used to estimate the 96-h EC50 was: Log 96-hEC50 = -0.548 - 0.434 log Kow  
: ECOSAR Program (v0.99g) 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-

CAS Num: 000102-60-3

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C14 H32 N2 O4

MOL WT : 292.42

Log Kow: -2.08 (KowWin estimate)

Melt Pt:

Wat Sol: 1.886E+007 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

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Aliphatic Amines

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
=====	=====	=====	=====	=====
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	1.41e+006
Aliphatic Amines	: Fish	96-hr	LC50	32901.113
Aliphatic Amines	: Daphnid	48-hr	LC50	1434.599
Aliphatic Amines	: Green Algae	96-hr	EC50	661.806
Aliphatic Amines	: Green Algae	96-hr	ChV	57.774

Note: \* = asterick designates: Chemical may not be soluble enough to measure this predicted effect.

Fish and daphnid acute toxicity log Kow cutoff: none

Green algal EC50 toxicity log Kow cutoff: none

Chronic toxicity log Kow cutoff: none

MW cutoff: none

### Reliability

21.06.2004

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

## 5.1.1 ACUTE ORAL TOXICITY

<b>Type</b>	:	LD50
<b>Value</b>	:	= 11200 mg/kg bw
<b>Species</b>	:	rat
<b>Strain</b>	:	
<b>Sex</b>	:	male
<b>Number of animals</b>	:	10
<b>Vehicle</b>	:	water
<b>Doses</b>	:	4400, 5600, 7500, 9750, 12600, 16500 mg Quadrol/kg
<b>Method</b>	:	other: study pre-dates standardized methods
<b>Year</b>	:	1956
<b>GLP</b>	:	no
<b>Test substance</b>	:	
<b>Method</b>	:	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.
<b>Reliability</b>	:	(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

<b>Type</b>	:	Sub-acute
<b>Species</b>	:	rat
<b>Sex</b>	:	male/female
<b>Strain</b>	:	other: Harlan albino
<b>Route of admin.</b>	:	oral feed
<b>Exposure period</b>	:	three months
<b>Frequency of treatm.</b>	:	ad libitum
<b>Post exposure period</b>	:	no post-exposure observation period
<b>Doses</b>	:	Doses were equivalent to average daily intakes of 70, 210, 720, 2170 and 3750 mg/kg bw
<b>Control group</b>	:	yes, concurrent no treatment
<b>NOAEL</b>	:	ca. 600 900 mg/kg
<b>Method</b>	:	
<b>Year</b>	:	1956
<b>GLP</b>	:	no
<b>Test substance</b>	:	
<b>Method</b>	:	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.
<b>Result</b>	:	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

## 5. Toxicity

Id 102-60-3

Date 29.06.2004

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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 29.06.2004

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- (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.

201-15441B<sub>2</sub>

# I U C L I D

## Data Set

2004 JUL 12 PM 12: 06

RECEIVED  
OPPT/CEIC

**Existing Chemical** : ID: 122-20-3  
**CAS No.** : 122-20-3  
**EINECS Name** : 1,1',1"-nitriлотрипропан-2-ол  
**EC No.** : 204-528-4  
**TSCA Name** : 2-Propanol, 1,1',1"-nitriлотрис-  
**Common name** : triisopropanolamine  
**Molecular Formula** : C<sub>9</sub>H<sub>21</sub>NO<sub>3</sub>

**Producer related part**  
**Company** : Arcadis  
**Creation date** : 02.10.2003

**Substance related part**  
**Company** : Arcadis  
**Creation date** : 02.10.2003

**Status** :  
**Memo** :

**Printing date** : 29.06.2004  
**Revision date** :  
**Date of last update** : 28.06.2004

**Number of pages** : 17

**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 29.06.2004

## 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

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. Physico-Chemical Data

Id 122-20-3

Date 29.06.2004

### 2.3 DENSITY

Type : density  
Value : = 1.01 g/cm<sup>3</sup> 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 29.06.2004

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. Environmental Fate and Pathways

Id 122-20-3  
Date 29.06.2004

#### 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 : = .000000000124029 cm<sup>3</sup>/(molecule\*sec)  
Degradation : 50 % after .1 day(s)

Method : APOWIN v1.91 (EPIWIN v3.11)  
Remark : assumed data: 1.5E6 OH/cm<sup>3</sup>; 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''-nitrotris-  
MOL FOR: C9 H21 N1 O3  
MOL WT : 191.27

----- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----  
Hydrogen Abstraction = 57.6090 E-12 cm<sup>3</sup>/molecule-sec  
Reaction with N, S and -OH = 66.4200 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Triple Bonds = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Olefinic Bonds = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Aromatic Rings = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Fused Rings = 0.0000 E-12 cm<sup>3</sup>/molecule-sec

OVERALL OH Rate Constant = 124.0290 E-12 cm<sup>3</sup>/molecule-sec  
HALF-LIFE = 0.086 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)  
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''-nitrotris-  
Molecular Wt: 191.27  
Henry's LC : 9.77e-012 atm-m<sup>3</sup>/mole (Henrywin program)  
Vapor Press : 1.86e-005 mm Hg (Mpbpwin program)  
Liquid VP : 6.31e-005 mm Hg (super-cooled)

### 3. Environmental Fate and Pathways

Id 122-20-3

Date 29.06.2004

Melting Pt : 78.6 deg C (Mpbwin program)  
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

### 3. Environmental Fate and Pathways

Id 122-20-3

Date 29.06.2004

of <5% using an unacclimated inoculum to 40-50% using an acclimated 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** : BASF AG Ludwigshafen  
24.11.2003

(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)

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

**Type** : static  
**Species** : Leuciscus idus (Fish, fresh water)  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**LC50** : > 2150  
**LC50** : < 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, 4640 and 10000 mg/L were used. To study the effect of the high pH on toxicity, the highest test concentration was tested in parallel after pH adjustment. Ten fish were exposed to each test concentration. The fish ranged in length from 5.3 to 6.3 cm, with an average of 5.7 cm, and ranged in weight from 2.2 to 3.9 g with an average of 2.8 g. The age of the test fish was not reported. Fish were held for approximately 6 weeks after receipt from the supplier. Mortality and any abnormal symptoms were observed at 1, 4, 24, 48, 72 and 96 hours of exposure

**Result** : Initial pH ranged from 8.1 in the control to 10.0 in the 10000 mg/L test concentration; final pH ranged from 8.0 in the control to 9.7 in the 10000 mg/L test concentration. Initial dissolved oxygen was 8.2 or 8.3 mg/L in all test concentrations; final dissolved oxygen ranged from 8.2 mg/L in the 2150 mg/L test concentration to 8.9 mg/L in the 10000 mg/L test concentration. Temperature was 20 degrees Centigrade in all test concentrations at all 24-h measurement intervals.

All fish exposed to the highest concentration died within 24 hours. At 96 hours, mortality was 0/10, 0/10, 0/10, 10/10, and 10/10 for the control, 1000 mg/L, 2150 mg/L, 4640 mg/L and 10000 mg/L test concentrations, respectively. In the pH-adjusted 10000 mg/L test solution, mortality was 10 out of 10 at 96 hours. The 96-h LC50 was between 2150 and 4640 mg/L, as determined using probit analysis. The NOEC was 2150 mg/L.

**Source** : BASF AG Ludwigshafen  
**Test condition** : Test concentrations were prepared in reconstituted fresh water, hardness 2.5 mmol/L, pH approx. 8.0. The test was conducted using a photoperiod of 16 hours light and 8 hours darkness. Temperature was 20 degrees Centigrade. Slight aeration was provided. Food was withdrawn from fish 1 day prior to exposure. Loading of fish was 2.8 g per liter of test water.

**Reliability** : (1) valid without restriction  
 Test conducted according to standard procedure and with appropriate documentation.

28.06.2004

(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

## 4. Ecotoxicity

Id 122-20-3

Date 29.06.2004

**EC100** : > 500  
**Analytical monitoring** : no  
**Method** : other: Directive 79/831/EEC, Annex V, Part C  
**Year** : 1988  
**GLP** : no  
**Test substance** : other TS: triisopropanolamine, purity not reported

**Method** : Seven test concentrations (7.81, 15.6, 31.2, 62.5, 125, 250 and 500 mg/L) and a control were used. Four replicates were used at each concentration, with 5 animals per replicate for a total of 20 animals per test concentration. The age of the test organisms was 2 - 24 hours old. Immobilization was observed at 0, 3, 6, 24 and 48 hours of exposure.

**Result** : The number of immobile organisms after 48 hours was: 0/20, 0/20, 0/20, 0/20, 0/20, 0/20, 0/20 and 3/20 in the control, 7.81, 15.6, 31.2, 62.5, 125, 250 and 500 mg/L test concentrations, respectively. The initial pH ranged from 8.01 in the control to 9.05 in the 500 mg/L test concentration, and the final pH ranged from 7.56 in the control to 8.35 in the 500 mg/L test concentration. The initial dissolved oxygen ranged from 8.60 in the control to 8.79 in the 250 mg/L test concentration, while the final dissolved oxygen ranged from 8.23 in the 250 mg/L test concentration to 8.94 mg/L in the 7.81 mg/L test concentration.

Effect values after 24 h and 48 hours were the same. Expressed as the nominal concentrations:

EC0 (24 h): =250 mg/L  
EC50 (24 h): >500 mg/L  
EC100 (24 h): >500 mg/L

No statistical methods were employed (due to lack of sufficient immobilization to calculate EC50).

**Source** : BASF AG Ludwigshafen  
**Test condition** : Tests were conducted in water with a pH of 7.9, hardness of 2.77 mmol/L, and conductivity of 550 - 650 microSiemens/cm. The temperature was 291 - 293 degrees Kelvin (18 - 20 degrees Celsius) and the photoperiod was 16 hours light and 8 hours dark.

**Reliability** : (1) valid without restriction  
Test conducted according to standard procedure and with appropriate documentation.

28.06.2004

(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  
**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 %

**Method** : The test was conducted using OECD medium with a conductivity of 8.03 microSiemens/cm and a pH of 9.63. An initial algal inoculum of 10,000 cells/mL was exposed at each of 7 test concentrations and a control. The

<b>Remark</b>	<p>nominal test concentrations were control, 1.562, 3.125, 6.25, 12.5, 25, 50 and 100 mg/L. In addition, a neutralized 100 mg/L treatment was tested to examine the effects of pH on toxicity. Tests were conducted using 100 mL of test solution in 250 mL Erlenmeyer flasks, with 4 replicates per test treatment, at 293 degrees Kelvin (20 degrees Celsius). Light intensity and quality were not reported. Fluorescence was measured in each test vessel at 24, 48 and 72 hours.</p> <p>: 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 &gt; 100 mg/L</p> <p>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:</p> <p>ErC10 = 16.1 mg/L            ErC50 &gt; 100 mg/L            ErC90 &gt; 100 mg/L</p> <p>and biomass values of:            EbC10 = 8.84 mg/L            EbC50 = 68.93 mg/L            EbC90 &gt; 100.0 mg/L</p>
<b>Result</b>	<p>The most sensitive results are those based upon biomass.</p> <p>: Effect values related to nominal concentration of the test substance. Results are based upon measurement of fluorescence as a surrogate for cell density, which was subsequently recalculated to reflect growth rate and biomass as explained above. At 72 hours, the percent fluorescence, compared to the control, was:            100% at 1.562 mg/L            97% at 3.125 mg/L            87% at 6.25 mg/L            76% at 12.5 mg/L            55% at 25 mg/L            43% at 50 mg/L            40% at 100 mg/L            57% at the neutralized 100 mg/L</p>
<b>Source Reliability</b>	<p>Statistical methods used to calculate EC values were not reported.</p> <p>: BASF AG Ludwigshafen            : (1) valid without restriction            test procedure according to National Standard (German Industrial Standard DIN)</p>
28.06.2004	(11) (12)

#### 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

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

## 4. Ecotoxicity

Id 122-20-3  
Date 29.06.2004

**GLP** : no  
**Test substance** :

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

**Source** : BASF AG Ludwigshafen  
03.09.2003 (7)

**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.

## 5. Toxicity

Id 122-20-3

Date 29.06.2004

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<b>Test condition</b>	: Test conditions not described in English	
<b>Reliability</b>	: (4) not assignable Insufficient documentation	
22.10.2003		(15)
<b>Type</b>	:	
<b>Species</b>	: rat	
<b>Sex</b>	: male/female	
<b>Strain</b>	: no data	
<b>Route of admin.</b>	: drinking water	
<b>Exposure period</b>	: 30 days	
<b>Frequency of treatm.</b>	: continuously in the drinking water	
<b>Post exposure period</b>	: no data	
<b>Doses</b>	: 140 mg/kg - 1350 mg/kg	
<b>Control group</b>	: yes, concurrent no treatment	
<b>NOAEL</b>	: 140 mg/kg	
<b>Method</b>	: other	
<b>Year</b>	:	
<b>GLP</b>	: no	
<b>Test substance</b>	:	
<b>Method</b>	: Animals (5 per dose) were exposed to triisopropanolamine in the drinking water for 30 days.	
<b>Result</b>	: 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.	
<b>Reliability</b>	: (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'

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

### 5.6 GENETIC TOXICITY 'IN VIVO'

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

## 5. Toxicity

Id 122-20-3

Date 29.06.2004

**Result** :  
**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

## 5. Toxicity

Id 122-20-3

Date 29.06.2004

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<b>NOAEL maternal tox.</b>	:	400 mg/kg bw
<b>NOAEL teratogen.</b>	:	>= 1000 mg/kg bw
<b>Method</b>	:	OECD Guide-line 414 "Teratogenicity"
<b>Year</b>	:	
<b>GLP</b>	:	yes
<b>Test substance</b>	:	other TS
<b>Result</b>	:	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.
<b>Source</b>	:	BASF AG Ludwigshafen
<b>Test substance</b>	:	Triisopropanolamine, purity 92 %
22.10.2003		

(20)

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

<b>Type</b>	:	
<b>In vitro/in vivo</b>	:	In vivo
<b>Species</b>	:	rat
<b>Sex</b>	:	male
<b>Strain</b>	:	Wistar
<b>Route of admin.</b>	:	oral feed
<b>Exposure period</b>	:	102 weeks
<b>Frequency of treatm.</b>	:	
<b>Duration of test</b>	:	102 weeks
<b>Doses</b>	:	Single dose, approximately equal to 1216 mg/kg bw/day
<b>Control group</b>	:	yes, concurrent no treatment
<b>Method</b>	:	other: study was designed to examine carcinogenic effects
<b>Year</b>	:	1991
<b>GLP</b>	:	no data
<b>Test substance</b>	:	
<b>Method</b>	:	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.
<b>Result</b>	:	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.
<b>Test condition</b>	:	Test conditions not described in English
<b>Reliability</b>	:	(4) not assignable Insufficient documentation
16.10.2003		

(15)

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  - (4) BASF AG, Analytisches Labor; unveroeffentlichte Untersuchung, BRU 87.262, 18.12.1987
  - (5) BUA, Triisopropanolamine, BUA Report 148. German Chemical Society (GDCh) - Advisory Committee on Existing Chemicals of Environmental Relevance (BUA). (1993)
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  - (18) BASF AG, dept. of toxicology, unpublished data (26M0013/9[C196), 02/23/1995
  - (19) Toropkov V.V.: Tr. Leningr. San.-gigien Med.In-ta 130, 29 (1980). cited in: BIBRA Toxicity Profile "Triisopropanolamine" (1990)
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