AR201-13378B

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE . . . . . CHEMICAL

Benzenamine, N-phenyl-, reaction product with 2,4,4-trimethylpentene

CAS No. 68411 - 46 - 1

RECEIVED
OPPT NCIC
2001 DEC 20 AM 10:45

Name of Sponsoring Organization: Rubber and Plastic Additives Panel
Technical Contact Person: Anne LeHuray
American Chemistry Council

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. Cast number** 68411-46-1

B. Name *(IUPAC name)*

***C. Name** *(OECD name)* .....

†D. CAS Descriptor *(where applicable for complex chemicals)*

Benzenamine, N-phenyl-, reaction product with 2,4,4-trimethylpentene

E. EINECS-Number 270 -128 - 1

F. Molecular Formula .....

***G. Structural Formula** *(indicate the structural formula in smiles code, if available)*

.....

H. Substance Group *(if possible, only for petroleum products, see HEDSET explanatory note)*

.....

I. Substance Remark *(Indicate the substance remark as prescribed in the EINECS Inventory, if possible)*

.....

J. Molecular Weight 298-350 .....

1.02 OECD INFORMATION

A. Sponsor Country: .....

B. Lead Organisation:

Name of Lead Organisation: BFGoodrich.....
Contact person: Robert K. Hinderer, Ph.D. .....
Address:
Street: 9911 Brecksville Road .....
Postal code: 44141-3247.....
Town: Cleveland, Ohio .....
Country: U.S.A.....
Tel: (216) 447-5181.....
Fax: (216) 447-5710.....

C. **Name of responder** *(Information on a responder should be provided when companies respond to Lead Organisation or SIDS Contact Points.)*

Name: .....
Address: .....
Street: .....
Postal code: .....
Town: .....
Country: .....
Tel: .....
Fax: .....

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [x]; organometallic [ ];
petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [x]; solid **[ ]**

C. Purity *(indicate the percentage by weight/weight)* .....

1.2 SYNONYMS Vanlube® 848; Naugalube® 640 .....
.....
.....
.....
.....

1.3 IMPURITIES *[Indicate CAS No., chemical name (IUPAC name is preferable), percentage, if possible EINECS number.]*

CAS No: 122-39-4
EINECS No: .....
Name: Diphenylamine .....
Value: 3-5% .....
Remarks: BFGoodrich Vanlube® 848 .....

1.4 ADDITIVES *(e.g. stabilising agents, inhibitors etc. Indicate CAS No., chemical name (IUPAC name is preferable), percentage, if possible EINECS number), the component of the UVCB (substance with no defined composition) should be indicated here.*)

CAS No: . . . . . - . . . . . - . . . . . .
EINECS No: . . . . . - . . . . . - . . . . . .
Name: .....
Value: .....
Remarks: .....

2. PHYSICAL-CHEMICAL DATA

***2.1 MELTING POINT** *(If more than one, identify the recommended value.)*

Value: 44-107. . . . . .°C
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updated of the method used)]*
. .....
GLP: Yes **[ ]** No **[x]** ? **[ ]**
Remarks: Range for major components; the melting point of the butylated/octylated component could not be determined because it was an oil.
Reference: BFGoodrich Laboratory. .....

***2.2 BOILING POINT** *(If more than one, identify the recommended value.)*

Value: >300. . . . . °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: >200° C (BFGoodrich and Uniroyal MSDS's). .....
Reference: Ciba MSDS. .....

BOILING POINT *(If more than one, identify the recommended value.)*

Value: Approx. 370. . . . . °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: 326.04 to 431.62 for major components.....
Reference: EPIWIN

†2.3 DENSITY (relative density) *(Where applicable, indicate the relative density of the substance.)*

Type: Bulk density **[ ]**; Density **[x]**; Relative Density **[ ]**
Value: 0.97 +/- 0.01 mg/m3.....
Temperature: 25. . . . . °C
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Remarks: Specific Gravity 0.96-0.99 (H20=1) (Ciba MSDS) .....
Reference: BFGoodrich MSDS.....

***2.4 VAPOUR PRESSURE** *(if more than one, identify the recommended value)*

Value: 2x10(-5) mmHg. . . . . hPa

Temperature: 25. . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updated of the method used)].
. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Negligible @ 20 degrees C (Uniroyal MSDS). .....
Reference: Ciba MSDS .....

VAPOUR PRESSURE *(if more than one, identify the recommended value)*

Value: 1.14E-004 to 5.05E-008. . . . . hPa
Temperature: . . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updated of the method used)].
EPIWIN. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Range for major components .....
Reference: EPIWIN

***2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$** *(if more than one, identify the recommended value)*

Log Pow: >>6.
Temperature: . . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)].
. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: . .....
Reference: Ciba MSDS. .....

PARTITION COEFFICIENT $\log_{10}P_{ow}$ *(if more than one, identify the recommended value)*

Log Pow: 5.2 to 10.82. . . . . .
Temperature: . . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)].
EPIWIN. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Range for major components. .....
Reference: EPIWIN

***2.6 WATER SOLUBILITY** *(if more than one, identify the recommended value)*

A. Solubility

Value: <0.01%. . . . . .
Temperature: 20. . . . . °C

Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Negligible (BFGoodrich MSDS; Insoluble in water (Uniroyal MSDS). .....

Reference: Ciba MSDS. .....

Solubility

Value: 1.167 to 1.939e-006 mg/l. . . . . .
Temperature: . . . . . °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Range for major components. .....
Reference: EPIWIN.....

B. pH Value, pKa Value

pH Value: . . . . . .
Concentration: . . . . . .
Temperature: . . . . . °C
Method: *[e.g. OECD, other (with the year of publication or updating of the method used).*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
(Where applicable, enter values for the dissociation constant(s) and the conditions under which they were measured.)
pKa value . . . . . at 25°C
Remarks: . .....
Reference: . .....

2.7 FLASH POINT *(liquids)*

Value: . . . . . °C
Type of test: Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**
Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.8 AUTO FLAMMABILITY *(solid/gases)*

Value: . . . . . °C
Pressure: . . . . . hPa
Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.9 FLAMMABILITY

Results: Extremely flammable **[ ]**; Extremely flammable - liquified gas **[ ]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.10 EXPLOSIVE PROPERTIES

Results: Explosive under influence of a flame**[ ]**;
More sensitive to friction than m-dinitrobenzene **[ ]**;
More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**;
Other **[ ]**
Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;
Vigorous reaction in preliminary test **[ ]**;
No oxidising properties **[ ]**; Other **[ ]**

Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

†2.12 OXIDATION: REDUCTION POTENTIAL

(Where applicable, indicate the redox potential and the conditions under which it was measured.)

Value: . . . . . mV
Method: *(with the year of publication or updating of the method used)*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value: . . . . . .
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

B. Other data

(e.g. Henry's Law constant, fat solubility, surface tension (of aqueous solution), adsorption/desorption on soil, particle size distribution, etc.)

Results: . .....
Remarks: . .....
Reference: . .....

3. ENVIRONMENTAL FATE AND PATHWAYS

[Reporting of studies should give the test method, test conditions (laboratory versus field studies), test results (e.g. % degradation in specified time period) and reference. Information on breakdown products (transient and stable) should be provided when available.]

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air **[x]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: . . . . . nm
Relative intensity: . . . . . *(based on intensity of sunlight)*
Spectrum of substance: *[e.g. lambda (max.)(>295nm) and epsilon (max) or epsilon (295nm)]*
. . . . . nm
Concentration of Substance: . . . . . .
Temperature: . . . . . °C
Direct photolysis:
Half life: 0.053 days. . . . . .
Degradation: . . . . . % (weight/weight) after . . . . . (exposure time)
Quantum yield: . . . . . .
Indirect Photolysis:
Type of sensitizer: . . . . . .

Concentration of sensitizer: . . . . . .
Rate constant (radical): . . . . . cm^3/molecule*sec
Degradation: . . . . . .

Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)]
EPIWIN

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity:. . . . . .

Remarks: Range for major components .....

Reference: EPIWIN.....

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**

Half life: . . . . . at pH . . . . . at . . . . . °C

Degradation: . . . . . at pH . . . . . at . . . . . °C after
. . . . . (exposure time)

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* . HYDROWIN Program (v. 1.67).....
. .....

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: N-Phenylbenzeneamine, reaction products with 2,4,4-trimethylpentene
CAS No. 68411-46-1
purity: . . . . . .

Remarks: *(e.g. CAS number, name and percentage of degradation products)*
No estimate available; This program cannot estimate a hydrolysis rate for this type of structure.

Reference Syracuse Research Corporation, Syracuse, NY; Pollution Prevention (P2) Assessment Framework, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics (Draft), 1998

3.1.3 STABILITY IN SOIL

Type : Field trial **[ ]**; Laboratory **[ ]**; Other **[ ]**

Radiolabel: Yes **[ ]** No **[ ]** ? **[ ]**

Concentration: . . . . . .

Soil temperature: . . . . . °C

Soil humidity: . . . . . .

Soil classification: DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[ ]**
year . . . . . .

Content of clay etc.: Clay . . . . . %, Silt . . . . . %, Sand . . . . . %

Organic Carbon: . . . . . .

Soil pH: . . . . . .

Cation exchange capacity: . . . . . .

Microbial biomass: . . . . . .

Dissipation time: DT 50 : . . . . . .
DT 90 : . . . . . .

Dissipation : . . . . . % after . . . . . (time)

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

*3.2 MONITORING DATA (ENVIRONMENTAL)

Note that data on biological effects monitoring, including biomagnification, and biotransformation and kinetics in environmental species are to be reported in section 4.7 and 4.8, respectively. Nonetheless, concentration in various biota should be reported here. Data on concentration in the workplace or indoor environment should be reported under item 5.11.

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**
Media: . .....
Results: . .....
Remarks: . .....
Reference: . .....

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS *(e.g. during the chemical life-cycle. The information should indicate whether the calculation is on a global basis or is site-specific, and whether it is based on laboratory measurements or field observations.)*

*3.3.1 TRANSPORT

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media: . .....
Method: .....
Results:

Remarks:

.

Reference:
.

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**; Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**
Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[x]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**
EPIWIN. .....
Results: Air 0.0697%, 1.28 hr half-life, 1000 kg/hr

Water 17.4%, 900 hr half-life, 1000 kg/hr
Soil 49.6%, 900 hr half-life, 1000 kg/hr
Sediment 33%, 3.6e+003 hr half-life, 1000 kg/hr. .....

Remarks: . .....

Reference: EPIWIN.....

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

Results: . .....

Remarks: . .....

Reference: . .....

*3.5 BIODEGRADATION

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[ ]**; . Fresh sewage treatment plant sample (per guideline)

Concentration of the chemical: related to COD **[ ]**; DOC **[ ]**; test substance **[ ]** Reference substance, Aniline, Merck No.: 1261, 20 mg/ L and
Test substance: 10.6 mg/ L, and 20.1 mg/ L.

Medium: water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ];** Sewage sludge (per guideline)

Degradation: *(percentage reduction/exposure time)*
. . . . . % after . . . . . (time)

Results: *(see OECD Guidelines)* readily biodeg. **[ ];** inherently biodeg. **[ ];** under test condition no biodegradation observed **[X]**, other **[ ];** Biodegradation:
Test substance : 10.6 mg/L = 0 % after 28 days
20.1 mg/L = 1 % after 28 days

Under the test conditions, no biodegradation was observed.

Kinetic (e.g. Zahn-Wellens-Test) . . . . . % in . . . . . (time)

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. OECD Guideline 301 B. Bacteria collected from activated sludge of the sewage treatment plant of CH - 4153 Reinach on 18/08/88. The preparation was carried out according to the method described in the guideline, with the exception that the volume of test solution was reduced from 3 to 1.5L
. .....

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: N-Phenylbenzeneamine, reaction products with 2,4,4-trimethylpentene
CAS No. 68411-46-1
Batch No. EN 139 879.82
purity: . . . . . .

Remarks: *[In the case of poorly soluble chemicals, treatment given (nature, concentration, CAS number, name and percentage of degradation products etc.)]:*. This study is assigned a reliability code of 2b (guideline study with acceptable restrictions) according the criteria established by Klimisch *et al* (1997).

. .....

Reference: Report on the Test for Ready Biodegradability of TK 12340 in the Modified Sturm Test, OECD- GUIDELINE No. 301 B (Paris 1981), Project No: 88 42 49; Dr. A. de Morsier, U. Bader, 10/04/88, CIBA - GEIGY Ltd., Basle, Switzerland. 1988.

.

3.6 BOD$_5$, COD OR RATIO BOD$_5$/COD

BOD$_5$

Method: . . . . . .

Concentration: . . . . . related to COD **[ ]**; DOC **[ ]**; Test substance **[ ]**

Value: . . . . . mg O_2/l

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

COD

Method: . . . . . .

Value: . . . . . mg O_2/g

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Ratio BOD$_5$/COD: . . . . . .

Remarks: . .....

Reference: . .....

3.7 BIOACCUMULATION

Species: . .....

Exposure period: . .....

Temperature: . . . . . °C

Concentration: . . . . . .

BCF: . . . . . .

Elimination: Yes **[ ]** No **[ ]** ? **[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.

. .....

Type of test: calculated **[ ]**; measured **[ ]**

static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity:. . . . . .

Remarks: . .....

Reference: . .....

3.8 ADDITIONAL REMARKS

A. Sewage treatment *(information on treatability of the substance)*

Results: .....
Remarks: .....
Reference: .....

B. Other information *[information that will help to focus the exposure assessment (either qualitative or quantitative)]*

Results: .....
Remarks: .....
Reference: .....

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species: Zebra Fish (Brachydanio rerio)

Exposure period: 96 hrs.....
Results: LC_{50} (96 h):

* Based on mean measured concentrations.

Nominal mg/L	day 1 mg/L	day 4 mg/L	Mean Measured mg/L	%. Dead (10 per conc.)
10	6	2.9	4.45	0
18	9.6	3.8	6.7	0
32	19.6	9.1	14.35	0
58	41.3	16	28.65	0
100	70.8	23.3	47.05	40

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. OECD Guideline No. 203 (Paris 1984). Highest vehicle concentration: 950.8 mg/l. Due to insolubility of test substance a stock solution was prepared as follows: 5 g of TK 12340 was mixed with 40.0 mg alkylphenol-polyglycol-ether and made up to 50 ml with DMF.

.....
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: N-Phenylbenzeneamine, reaction products with 2,4,4-trimethylpentene
CAS No. 68411-46-1
Batch No. EN-127 506.82
purity: . . . . . .

Remarks: 10 fish per concentration and control.
10 fish per aquarium.
Supplier: West-Aquarium, D-3422 Bad Lauterberg
Length: 25 mm (21- 30 mm)
Weight: 0.15g (0.08 - 0.25 g)
Loading: 0.10 g/L
Concentrations of 10, 18, 32, 58 and 100 mg/L (nominal)
This study is assigned a reliability code of 2b (guideline study with acceptable restrictions) according the criteria established by Klimisch *et al* (1997).

Reference: Report on the test for acute toxicity of TK 12340 to Zebra Fish, OECD-Guideline No. 203, Paris 1984, Project No. 884252; Dr. A. de Morsier, Dr. H. Rufli; Dr. U. Bader; 09/06/88, Ciba-Geigy Limited, Basle, Switzerland. 1988.

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test: static **[x]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: Daphnia Magna Straus 1820. .....
Exposure period: 24 hrs.....
Results: EC_{50} (24 h) : 0.82 mg/L* (95% Conf. Interval 0.72 - 0.98 mg/L)
*based on mean measured concentration

Analytical monitoring: Yes **[x]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. OECD Guideline No. 202 (Paris 1984)
. .....
GLP: Yes **[ ]** No **[x]** ? **[ ]**
Test substance: N-Phenylbenzeneamine, reaction products with 2,4,4-trimethylpentene
CAS No. 68411-46-1
Batch No. EN- 127 506.82, purity: . . . . . .
Remarks: Analytical data of test concentrations.

Concentrations nominal, mg/L	Measured Concentrations				Mean (0 h/ 24 h) mg/L	% Daphnia Immobile
	Initial (0 h)		End (24 h)			
	mg/L	% Nominal	mg/L	% Nominal		
0.18	n.d.		n.d.		-	0
0.32	0.4	125	0.3	94	0.35	0
0.58	0.8	138	0.5	86	0.65	5
1.0	0.6	60	0.5	50	0.55	55
1.8	1.2	67	1.1	61	1.15	70
3.2	2.3	72	1.8	56	2.05	100

n.d. : not determined

The study is assigned a reliability code of 2C (comparable to guideline study with acceptable restrictions).

Reference: Report: Test for acute Toxicity of TK 12340 to Daphnia magna; OECD-Guideline No. 202, Paris 1984; Project No.: 884250; Drs. A. De Morsier, H. Rufli, Dr. U. Bader; CIBA- GEIGY Ltd., Basle, Switzerland. 1988.

.

B. Other aquatic organisms

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: .....
Exposure period: .....
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (..h) = ... mg/l
NOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

***4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae**

Species: .....
Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[ ]**
Exposure period: .....
Results: . . . . . EC_{50} (. . . . . .h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . .h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....
.....
open-system **[ ]**; closed-system **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

4.4 TOXICITY TO BACTERIA *(Single species tests and tests on overall processes such as nitrification or soil respiration are included in this item.)*

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: . .....
Exposure Period: . .....
Results: EC_{50} (. . . h) = ... mg/l
EC_{xx} (. . . h) = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH (*effects on reproduction, embryo/larva, etc.*)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[ ]**
Exposure period: . .....
Results: . . . . . EC_{50} (..d) = ... mg/l
(Endpoint) EC_{xx} (..d) = ... mg/l
NOEC = ...mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

(*)4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES *(e.g. daphnia reproduction. The need to conduct tests for this endpoint will depend inter alia upon possible concern for long term effects.)*

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: .....
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period: . . . . . .
Results: . . . . . EC_{50} (. . . . . h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . d) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[ ]**
Species: .....
Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period: .....
Results: . . . . . EC_{50} (. . . . . d) = ... mg/kg
(Endpoint) EC_{50} (. . . . . d) = ... mg/kg
EC_{xx} (. . . . . d) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)

Species: .....

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**

Exposure period: .....

Results: EC_{50} and/or LC_{50} (7d) = ... mg/l

EC_{50} and/or LC_{50}(14d) = ... mg/l

EC_{xx} and/or LC_{xx} (xxd) = ...mg/l

NOEC = ...mg/l

LOEC = ...mg/l

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....

.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

(b)

Species: .....

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**

Exposure period: .....

Results: EC_{50} and/or LC_{50} (7d) = ... mg/l

EC_{50} and/or LC_{50}(14d) = ... mg/l

EC_{xx} and/or LC_{xx} (xxd) = ...mg/l

NOEC = ...mg/l

LOEC = ...mg/l

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....

.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

(c)

Species: ..... .

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**

Exposure period: .....

Results: EC_{50} and/or LC_{50} (7d) = ... mg/l

EC_{50} and/or LC_{50}(14d) = ... mg/l

EC_{xx} and/or LC_{xx} (xxd) = ...mg/l

NOEC = ...mg/l

LOEC = ...mg/l

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....

.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species: . .....
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period: . .....
Results: LD_{xx} or LC_{xx} (xxd) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:....., purity: .....
Remarks: . .....
Reference: . .....

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

(Studies on variation of predominant species in certain ecosystems (e.g. mesocosm) and monitoring of biological effects are included.)

Results: Substance:.....
Species or ecosystem studied: .....
Effects monitored: .....
Results:.....
Chemical analysis:.....
Remarks: *(Information on environmental conditions (e.g. water characteristics: suspended matter, pH, temperature, hardness; soil/sediment characteristics: % organic matter, clay content)*
.....
Reference: .....

4.8 BIOTRANSFORMATION AND KINETICS

(Under this item, studies on absorption, distribution, metabolism and excretion etc. should be given.)

Type: Animal **[ ]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Results: .....
Remarks: .....
Reference: .....

4.9 ADDITIONAL REMARKS

Results: .....
Remarks: .....
Reference: .....

5. TOXICITY

(Where observations on humans are available, these should be entered in the appropriate "Comments" section or under section 5.11.)

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[x]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: Rat, Tif : RAIf (SPF), F3- crosses of RII 1/Tif x RII 2/Tif strain. .....

Value: LD_{50} (males) > 5000 mg /kg bw
LD_{50} (females) > 5000 mg /kg bw.
LD_{50} (in both sexes) > 5000 mg /kg bw.

Disc

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* OECD Guideline No. 401.

.....

GLP: Yes **[ ]** No **[x]** ? **[ ]**

Test substance: N-Phenylbenzeneamine, reaction products with 2,4,4-trimethylpentene
CAS No. 68411-46-1
Batch No. EN 65360.22.368
purity: . . . . . .

Remarks: Sex: Males / Females
No. Animals/Group: 5 /sex / dose level
Initial Body weight range: 170 -221 g
Initial Age: 7-8 weeks
Distilled water containing 0.5% carboxymethylcellulose and 0.1% polysorbate 80

Dose Levels: Test substance: 5000 mg / kg
Vehicle: 10 ml/ kg body weight

Administration: Oral, gavage

Observation period: 14 days

TK 12340 has practically no acute toxicity when administered orally to the albino rat. The animals recovered within 13 days. No compound related gross organ changes were observed.

The study is assigned a reliability code of 2e. It was not conducted under GLP or OECD guidelines but generally meets scientific standards, is well documented and is accepted for assessment.

Reference: Report TK 12340 Acute Oral LD_{50} In The Rat, GU Project No: 821521; CIBA-GEIGY Ltd., Project-no. 821521; November 23, 1982; Dr. Phil II G Sarasin. 1982.

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**

Species/strain: .....

Exposure time: .....

Value: .....

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[x]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: Young Adult Albino Rats .....

Value: LD50>2000 mg/ kg bw

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[x]** ? **[ ]**

Test substance: N-Phenylbenzeneamine, reaction products with 2,4,4-trimethylpentene
Cas No: 68411-46-1
Batch No.: EN-127 506.82, purity: . . . . . .

Remarks: The exploratory acute dermal LD50 was estimated to be:
LD_{50} (males) > 2000 mg /kg bw
LD_{50} (females) > 2000 mg /kg bw.
LD_{50} (in both sexes) > 2000 mg /kg bw.

Clinical signs: Piloerection, abnormal body positions, and dyspnea were seen, being common symptoms in acute toxicity testing. The animals recovered within 9 days. At autopsy, no deviations from morphology were found.

The study is assigned a reliability code of 4. The study is essentially an abstract with minimal experimental details but confirms low acute toxicity as demonstrated orally (previous summary).

Reference: Summary Report TK 12340 Exploratory Acute Dermal Toxicity In The Rat; GU Project No: 884247; Dr. Phil H.R. Hartmann; Ciba - Geigy limited; Basle, Switzerland. 1988.

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION
(e.g. subcutaneous, intravenous, etc.)

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Route of Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time: .....
Value: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain: .....
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: *(If possible, according to EC Directive 67/548/EEC)*
Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[ ]**; Not irritating **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.2.2 EYE IRRITATION/CORROSION

Species/strain: .....
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.3 SKIN SENSITISATION

Type: Magnusson & Kligman Maximisation Test. .....
Species/strain: Guinea Pig/Dunkin Hartley.....
Results: Sensitizing **[ ]**; Not sensitizing **[x]**; Ambiguous **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Sensitizing **[ ]**; Not sensitizing **[x]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
OECD Guideline No. 406 referenced as Method B6 in Commision Directive 84/449/EEC (which consitutes Annex V of Council Directive 67/548/EEC)

GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance: Naugalube® 640. . . . . , purity: 99% . . . . . .
Remarks: . .....
Reference: Safepharm Laboratories, Inc./ Uniroyal Chemical Company, Inc. sponsor.

*5.4 REPEATED DOSE TOXICITY

Species/strain: . .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: . .....
Frequency of treatment: . .....
Post exposure observation period: .....
Dose: . .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL: . .....
LOEL: . .....
Results: . .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Reference: . .....

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: *(e.g. Bacterial reverse mutation assay, Bacterial gene mutation study, Cytogenetic Assay etc.)* Bacterial Mutagenicity (Ames)

.....

System of testing: Salmonella typhimurium, TA 98, TA 100, TA 1535 and TA 1537 .....

Concentration: The investigations were performed with the following concentrations of the trial substance with microsomal activation: 7.81, 15.6, 31.3, 62.5, 125, 250, 500 and 1000 ug/ ml and without microsomal activation: 19.5, 39.1, 78.1, 156, 313, 625, 1250 and 2500 ug/ ml.

Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[x]**; No data **[ ]**

Results:

Cytotoxicity conc: With metabolic activation: .....

Without metabolic activation: .....

Precipitation conc: .....

Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[x]**
Without metabolic activation:	**[ ]**	**[ ]**	**[x]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* This study was not conducted under OECD guidelines, but was conducted using the methods described by Ames *et al* (1973, 1975).

.....

GLP: Yes **[ ]** No **[x]** ? **[ ]**

Test substance: N-Phenylbenzeneamine, reaction products with 2,4,4-trimethylpentene
CAS No. 68411-46-1
Batch No.: EN - 127 506.82, purity: .....

Remarks: In the experiments performed with and without microsomal activation, treatment of the cultures with the various concentrations of TK 12340 did not lead to the formation of back- mutant bacteria. No evidence of the induction of point mutations by TK12340 or by the metabolites of the substance formed as a result of microsomal activation was detectable in the strains of S. Typhimurium used in these experiments.
This study is assigned a rating code of 2e (meets generally accepted scientific standards, well documented and accepted for assessment).

Reference: Salmonella Cobas Bact Pilot Test With TK 12340 (Irganox L 57) . (Test for mutagenic effects on bacteria); January 25, 1989; E. Deparade, Dr. P. Arni; CIBA-GEIGY Limited, Basel, Switzerland;1989.

B. NON-BACTERIAL IN VITRO TEST

Type: *(e.g. mammalian cell gene mutation assay, cytogenetic assay, etc.)*
. .....

System of testing: . .....

Concentration: . .....

Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[ ]**; No data **[ ]**

Results:

Cytotoxicity conc: With metabolic activation:. .....

Without metabolic activation:. .....

Precipitation conc: . .....

Genotoxic effects: + ? -

With metabolic activation: **[ ] [ ] [ ]**

Without metabolic activation: **[ ] [ ] [ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: . .....

Reference: . .....

* 5.6 GENETIC TOXICITY IN VIVO

Type: *(e.g. micronucleus assay, etc.)*
.....
Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: .....
Doses: .....
Results:
Effect on mitotic index or P/N ratio: .....
Genotoxic effects: + ? -
[ ] [ ] [ ]
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.7 CARCINOGENICITY

Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: .....
Frequency of treatment: .....
Postexposure observation period: .....
Doses: .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**; Other **[ ]**

Species/strain: .....

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Route of Administration:.....

Exposure period: .....

Frequency of treatment: .....

Post exposure observation period: .....

Premating exposure period: male: . . . . . , female: .....

Duration of the test: .....

Doses: .....

Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;

Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOEL Parental: .....

NOEL F1 Offspring: .....

NOEL F2 Offspring: .....

Results: .....

General parental toxicity:.....

Toxicity to offspring: *(weights of litter, postnatal growth, viability, etc.)*

.....

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....

.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species/strain: . .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: ..... .
Duration of the test: . .....
Exposure period: . .....
Frequency of treatment: . .....
Doses: . .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Maternal Toxicity: . .....
NOEL teratogenicity : . .....
Results: . .....
Maternal general toxicity: .....
Pregnancy/litter data: .....
Foetal data: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: *(e.g. neurotoxicity, immunotoxicity, etc.)*
. .....
Results: . .....
Remarks: . .....
Reference: . .....

B. Toxicodynamics, toxicokinetics

Type: *(e.g. toxicodynamics, toxicokinetics)*
. .....
Results: . .....
Remarks: . .....
References: . .....

I U C L I D

D a t a S e t

Existing Chemical	ID: 68442-68-2
CAS No.	68442-68-2
EINECS Name	Benzenamine,N-phenyl-, styrenated
EINECS No.	270-485-3

Producer Related Part	
Company:	Goodyear Chemicals Europe
Creation date:	05-APR-1998
Substance Related Part	
Company:	Goodyear Chemicals Europe
Creation date:	05-APR-1998

Printing date:	02-NOV-2001
Revision date:	
Date of last Update:	08-FEB-2001

Number of Pages:	10

Chapter (profile):	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8, 5.9
Reliability (profile):	Reliability: 1, 2
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 Melting Point

-

2.2 Boiling Point

-

2.4 Vapour Pressure

-

2.5 Partition Coefficient

log Pow: 4.64 at 22 degree C
Method: other (measured)
Year: 1990
GLP: yes
Reliability: (1) valid without restriction
27-JUL-2000 (1)

2.6.1 Water Solubility

Value: .41 mg/l at 20 degree C
Qualitative: of very low solubility
Method: Directive 84/449/EEC, A.6 "Water solubility"
Year: 1990
GLP: yes
Reliability: (1) valid without restriction
27-JUL-2000 (1)

3.1.1 Photodegradation
-

3.1.2 Stability in Water
-

3.3.1 Transport between Environmental Compartments
-

3.5 Biodegradation

Type:	anaerobic
Inoculum:	predominantly domestic sewage
Concentration:	100 mg/l related to Test substance
Degradation:	9 % after 28 day
Method:	other: OECD Guideline 30 C, modified according to EEC Round-robin-test "Assessment of Biodegradability of Chemicals in Water by Manometric Respiratory DGX 1/283/82 Rec. 5 EEC Directive 79/831 Annex V Part C"
Year:	1986 GLP: no
Test substance:	other TS
Test substance:	Batch No. C 40021 f 28.09.86
Reliability:	(2) valid with restrictions Although this study was not probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

27-JUL-2000 (1)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type:	static
Species:	Brachydanio rerio (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: no
LC0:	422
LC50:	920
LC100:	2400
Method:	other
Year:	1986 GLP: no
Test substance:	other TS
Remark:	Test substance dispersed in water by means of an Ultra-Turrax
Test substance:	Batch No. C 40021 of 28.08.86
Reliability:	(2) valid with restrictions Although this study was not probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

27-JUL-2000 (1)

4.2 Acute Toxicity to Aquatic Invertebrates
-

4.3 Toxicity to Aquatic Plants e.g. Algae
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain:
Sex: no data
Number of
Animals: 25
Vehicle: other: corn oil
Value: > 20000 mg/kg bw
Method: other
Year: 1976 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: The material was placed in a 25% corn oil solution and administered at dosages of 2500, 5000, 10000, 20000, and 40000 mg/kg to five rats each. The animals were observed for 14 days. Two of the five animals died at the dosages of 20000 and 40000 mg/kg.
Reliability: (2) valid with restrictions
Although this study was not probably not conducted to GLP, the test parameters used were based on a known and well established procedure for the time period.
31-JUL-2000 (5)

Type: LD50
Species: rat
Strain:
Sex: male/female
Number of
Animals: 10

Vehicle: other: corn oil
Value: > 500 mg/kg bw
Method: other: United States Department of Transportation Regulations, 49CFR173.132(1992)
Year: 1993 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Method: Five (5) male and five (5) female young adult rats (Sprague-Dawley, ZML:SD {MBM}) were administered a single dose of the test substance by gavage. The test substance was dispersed in corn oil at a dosage of 500 mg/kg. The animals were observed for clinical signs of toxicity at approximately 1-, 2.5- and 4-hours following administrations on the day of dosing and daily thereafter for 14-days. Body weights were recorded on Day-minus 1, Day-1, Day-7 and Day-14 of the study. All animals were subjected to a gross necropsy at study termination.
Result: No animals died during the 14-Day observation period. No significant clinical findings and no significant impairment on body weight gains were noted in either the male or female rats. No abnormal tissues were noted in any animals upon necropsy.
Reliability: (1) valid without restriction
27-JUL-2000 (9)

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 10000 mg/kg bw
Method: other
Year: 1976 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: No animals died after administration of 10000 mg/kg
Reliability: (2) valid with restrictions
Although this study was not probably not conducted to GLP, the test parameters used were based on a known and well established procedure for the time period.
31-JUL-2000 (3)

5.1.4 Acute Toxicity, other Routes
-

5.4 Repeated Dose Toxicity
-

5.5 Genetic Toxicity 'in Vitro'

Type:	other: Salmonella-Escherichia coli/Mammalian-Microsome Reverse Mutation Assay
System of testing:	Salmonella typhimurium (tester strains TA98, TA100, TA1535 and TA1537) and Escherichia coli (tester strain WP2uvrA)
Concentration:	33.3, 100, 333, 1000, 3300, and 5000 ug per plate
Cytotoxic Conc.:	
Metabolic activation:	with
Result:	negative
Method:	OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year:	2001 GLP: yes
Test substance:	as prescribed by 1.1 - 1.4
Method:	The objective of the study was to assess the potential of WINGSTAY 29 and/or its metabolites to induce reverse mutations in the presence and absence of a mammalian metabolic activation system with strains of Salmonella typhimurium and Escherichia coli strain WP2uvrA.

Based on results of a range-finding study with Salmonella typhimurium (tester starin TA100) and Escherichia coli (tester strain WP2uvrA), the doses for the test were 33.3, 100, 333, 1000, 3300 and 5000 ug per plate of WINGSTAY 29 in both the presence and absence of S9 metabolic activation. The assay used plate incorporation methodology. S. typhimurium strains TA98, TA100, TA1535 and TA1537, and the E. coli strain WP2uvrA were used. Following incubation, revertant colonies (mutations) were counted. The exogenous metabolic activation system was derived from Aroclor-induced Sprague-Dawley rat livers (S9). Dimethylsulfoxide (DMSO) was used as the vehicle for WINGSTAY 29. Vehicle and positive controls were included in the assay. All doses of WINGSTAY 29, the vehicle control, and positive controls were plated in triplicate.

The results of the initial assay were confirmed in an independent test.

No increase in the number of revertant colonies was seen in plates dosed with WINGSTAY 29 in the presence or absence of S9 metabolic activation in the initial and confirmatory

assays. All criteria for acceptable assays were met.
Result: WINGSTAY 29 did not cause reverse mutations in the S. typhimurium or E. coli tester strains in the presence or absence of metabolic activation system (rat liver S9).
Reliability: (1) valid without restriction
08-FEB-2001 (10)

Type: Ames test
System of testing: Salmonella typhimurium Strains TA-98, 100, 1535, and 1537
Concentration: 1, 10, 100, and 1000 micrograms/l
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1980 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: Test compound was evaluated for gnetic activity in the Ames test with and without the addition of mammalian metabolic activation.
Reliability: (2) valid with restrictions
Although this study was not probably not conducted to GLP, the test parameters used were based on a known and well established procedure.
08-FEB-2001 (13)

Type: Ames test
System of testing: Salmonella typhimurium Strains TA-98, 100, 1535, and 1537
Concentration: 10, 100, and 2000 micrograms/l
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1982 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: Test compound was evaluated for genetic activity in the Ames test with and without the addition of mammalian metabolic activation.
Reliability: (2) valid with restrictions
Although this study was not probably not conducted to GLP, the test parameters used were based on a known and well

established procedure.
08-FEB-2001 (14)

Type: DNA damage and repair assay
System of testing: Escherichia coli, Strains W 3110 (Pol A+) and p 3478 (Pol A1-)
Concentration: 10, 1000, 2500, and 5000 micrograms/l
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1981 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: A test for the ability of the chemical to damage cellular DNA in the E coli Pol A1- Liquid Suspension Assay
Reliability: (2) valid with restrictions
Although this study was not probably not conducted to GLP, the test parameters used were based on a known and well established procedure.
08-FEB-2001 (11)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse Sex: male
Strain: other: Crl:CD-1 (ICR) BR
Route of admin.: gavage
Exposure period: Single oral dose. Harvested 24 and 48 hours after dosing.
Doses: 0, 500, 1000 and 2000 mg/kg
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: 2001 GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Method: The objective of the study was to assess the potential of WINGSTAY 29 to induce chromosome damage in vivo in mice. The presence of micronuclei in polychromatic erythrocytes was used as an indicator of clastogenic activity and/or disruption of the mitotic apparatus.

Based on the results of a dose-finding assay, single doses of 0, 500, 1000, and 2000 mg/kg WINGSTAY 29 were administered to male Crl:CD-1 (ICR) BR mice. Corn oil was used as the vehicle. Five male mice per group were evaluated. Bone marrow cells were harvested 24 and 48 hours after dosing. All dose levels, the vehicle control and a positive control (Cyclophosphamide) were evaluated at the 24 hours. At 48 hours, only the vehicle control and high dose were evaluated.

Bone marrow was taken from the hind limbs. Slides were prepared from the bone marrow extracts, fixed with methanol and stained in May Grunwald Solution and Giemsa. Two thousand micronucleated polychromatic erythrocytes were evaluated for micronuclei. The ratio of polychromatic erythrocytes (PCE) to nonchromatic erythrocytes (NCE) cells was determined from the first 500 erythrocytes on each slide.

Wingstay 29 did not produce any signs of clinical toxicity. Statistically lower PCE:NCE ratios, while not dose related, did strongly indicate that WINGSTAY 29 was cytotoxic to the bone marrow. WINGSTAY 29 did not produce any statistically significant increase in micronucleated PCEs relative to the vehicle control at the 24-hour and 48-hour harvest interval. The positive control induced a statistically significant increase in micronucleated PCEs compared to the vehical control.

Result: Wingstay 29 was tested up to the limit dose (2000 mg/kg) and did not cause chromosome damage in the mouse bone marrow micronucleus assay under the conditions of this test.

Reliability: (1) valid without restriction

08-FEB-2001 (6)

5.8 Toxicity to Reproduction

-

5.9 Developmental Toxicity/Teratogenicity

-

6. References

(1) Bayer AG Data

(3) Food and Drug Research Laboratories, Inc., Acute Dermal Toxicity in Rabbits, Laboratory Report No. 2688b to The Goodyear Tire & Rubber Company, 1976

(5) Food and Drug Research Laboratories, Inc., The Acute Oral Toxicity in Rats, Laboratory Report No. 2688b to The Goodyear Tire & Rubber Company, 1976.

(6) In Vivo Mouse Micronucleus Assay with WINGSTAY 29, Reprt #; 21054-0-455OECD, Covance Laboratories (Vienna, Virginia), 1/19/01

(9) Ricerca Inc., Study No. 5797-93-0196-TX-000 to The Goodyear Tire & Rubber Company, 1993

(10) Salmonella-Escherichia coli/Mammalian-Microsome Reverse Mutation Assay with a Confirmatory Assay with WINGSTAY 29, Report #: 21054-0-409OECD, Covance Laboratories (Vienna, Virginia), 02/06/01

(11) The Goodyear Tire & Rubber Company, E. coli Pol A1- Liquid Suspension Assay on WINGSTAY 29, 1981.

(13) The Goodyear Tire & Rubber Company, Mutagenicity Evaluation of WINGSTAY 19, 1980.

(14) The Goodyear Tire & Rubber Company, Mutagenicity Evaluation of WINGSTAY 29, Laboratory Report No. 82-1-1, 1982.

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE . . . . . CHEMICAL

Benzenamine, N-phenyl-, reaction products with isobutylene and 2, 4, 4-trimethylpenetene

CAS No. 184378-08-3

Sponsor Country : . . . . . .

DATE: . . . . . .

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. Cast number** 184378-08-3

B. Name *(IUPAC name)* .....

***C. Name** *(OECD name)* .....

†D. CAS Descriptor *(where applicable for complex chemicals)*

Benzenamine, N-phenyl-, reaction products with isobutylene and 2, 4, 4-trimethylpente

E. EINECS-Number 270-128-1

F. Molecular Formula .....

***G. Structural Formula** *(indicate the structural formula in smiles code, if available)*

.....

H. Substance Group *(if possible, only for petroleum products, see HEDSET explanatory note)*

.....

I. Substance Remark *(Indicate the substance remark as prescribed in the EINECS Inventory, if possible)*

.....

J. Molecular Weight 225-393 .....

1.02 OECD INFORMATION

A. Sponsor Country: United States

B. Lead Organisation:

Name of Lead Organisation:
American Chemistry Council, Rubber and Plastic Additives (RAPA) HPV Panel

Street: 1300 Wilson Boulevard
Town: VA 22209 Arlington
Country: United States
Phone: 703-741-5600
Fax: 703-741-6091

C. **Name of responder** *(Information on a responder should be provided when companies respond to Lead Organisation or SIDS Contact Points.)*

Name: .....
Address: .....
Street: .....
Postal code: .....
Town: .....
Country: .....
Tel: .....
Fax: .....

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [x]; organometallic [ ];
petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [x]; solid **[ ]**

C. Purity *(indicate the percentage by weight/weight) 99 %*.....

1.2 SYNONYMS Good-rite® 3128NT

.....
.....
.....
.....

1.3 IMPURITIES *[Indicate CAS No., chemical name (IUPAC name is preferable), percentage, if possible EINECS number.]*

CAS No: 122-39-4
EINECS No: .....
Name: Diphenylamine .....
Value: <1%.....

Remarks: .....

1.4 ADDITIVES *(e.g. stabilising agents, inhibitors etc. Indicate CAS No., chemical name (IUPAC name is preferable), percentage, if possible EINECS number), the component of the UVCB (substance with no defined composition) should be indicated here.*)

CAS No: . . . . . - . . . . . - . . . . . .
EINECS No: . . . . . - . . . . . - . . . . . .
Name: .....
Value: .....
Remarks: .....

2. PHYSICAL-CHEMICAL DATA

***2.1 MELTING POINT** *(If more than one, identify the recommended value.)*

Value: 44-107. . . . . .°C
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updated of the method used)]*
. .....
GLP: Yes **[ ]** No **[x]** ? **[ ]**
Remarks: Range for major components; the melting point for the butylated/octylated component could not be determined because it is an oil.
Reference: BFGoodrich Laboroatory.....

***2.2 BOILING POINT** *(If more than one, identify the recommended value.)*

Value: >200 °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: BFGoodrich MSDS.....

BOILING POINT *(If more than one, identify the recommended value.)*

Value: Approx. 370 °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
.EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: .326.04 to 431.62 for major components.....
Reference: EPIWIN.....

†2.3 DENSITY (relative density) *(Where applicable, indicate the relative density of the substance.)*

Type: Bulk density **[ ]**; Density **[ ]**; Relative Density **[ ] Specific Gravity**
Value: Approx. 1
Temperature: . . . . . °C
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: BFGoodrich MSDS.....

***2.4 VAPOUR PRESSURE** *(if more than one, identify the recommended value)*

Value: 2x10(15)mmHg. . . . . hPa
Temperature: 25. . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updated of the method used)].
. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: .Components for this chemical are the same as for CAS# 68411-46-1; Uniroyal MSDS for CAS#68411-46-1 indicates negligible @20 degrees C
Reference: CIBA MSDS for CAS# 68411-46-1. .....

VAPOUR PRESSURE *(if more than one, identify the recommended value)*

Value: 1.14E-004 to 5.05E-008. . . . . hPa
Temperature: . . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updated of the method used)].
EPIWIN. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Range for major components. .....
Reference: .EPIWIN .....

***2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$** *(if more than one, identify the recommended value)*

Log Pow: >>6. . . . . .
Temperature: . . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)].
. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Components for this chemical are the same as for CAS# 69411-46-1. .....
Reference: CIBA MSDS for CAS# 68411-46-1. .....

PARTITION COEFFICIENT $\log_{10}P_{ow}$ *(if more than one, identify the recommended value)*

Log Pow: 5.2 to 10.82. . . . . .
Temperature: . . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)].
EPIWIN. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Range for major components.. .....
Reference: EPIWIN. .....

***2.6 WATER SOLUBILITY** *(if more than one, identify the recommended value)*

A. Solubility

Value: **Insoluble**. . . . . .
Temperature: . . . . . °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: BFGoodrich MSDS. .....

Solubility

Value: <0.01%. . . . . .
Temperature: . . . . . °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: .Components for this chemical are the same as for CAS# 68411-46-1. .....
Reference: CIBA MSDS. for CAS# 68411-46-1 .....

Solubility

Value: 1.167 to 1.939e-006 mg/l. . . . . .
Temperature: . . . . . °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
.EPIWIN .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: EPIWIN. .....

B. pH Value, pKa Value

pH Value: . . . . . .
Concentration: . . . . . .
Temperature: . . . . . °C
Method: *[e.g. OECD, other (with the year of publication or updating of the method used).*

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

(Where applicable, enter values for the dissociation constant(s) and the conditions under which they were measured.)

pKa value . . . . . at 25°C

Remarks: . .....

Reference: . .....

2.7 FLASH POINT *(liquids)*

Value: >180 °C

Type of test: Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**

Method: *(with the year of publication or updating of the method used).* .....
Pensky Martens. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: BFGoodrich MSDS (Flash range). .....

2.8 AUTO FLAMMABILITY *(solid/gases)*

Value: . . . . . °C

Pressure: . . . . . hPa

Method: *(with the year of publication or updating of the method used).* .....
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: . .....

2.9 FLAMMABILITY

Results: Extremely flammable **[ ]**; Extremely flammable - liquified gas **[ ]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**

Method: *(with the year of publication or updating of the method used).* .....
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: . .....

2.10 EXPLOSIVE PROPERTIES

Results: Explosive under influence of a flame**[ ]**;
More sensitive to friction than m-dinitrobenzene **[ ]**;
More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**;
Other **[ ]**

Method: *(with the year of publication or updating of the method used).* .....
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: .....
Reference: .....

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;
Vigorous reaction in preliminary test **[ ]**;
No oxidising properties **[ ]**; Other **[ ]**

Method: *(with the year of publication or updating of the method used).* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: .....
Reference: .....

†2.12 OXIDATION: REDUCTION POTENTIAL

(Where applicable, indicate the redox potential and the conditions under which it was measured.)

Value: . . . . . mV
Method: *(with the year of publication or updating of the method used)*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: .....
Reference: .....

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value: . . . . . .
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: .....
Reference: .....

B. Other data

(e.g. Henry's Law constant, fat solubility, surface tension (of aqueous solution), adsorption/desorption on soil, particle size distribution, etc.)

Results: .....
Remarks: .....
Reference: .....

3. ENVIRONMENTAL FATE AND PATHWAYS

[Reporting of studies should give the test method, test conditions (laboratory versus field studies), test results (e.g. % degradation in specified time period) and reference. Information on breakdown products (transient and stable) should be provided when available.]

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air **[x]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: . . . . . nm
Relative intensity: . . . . . *(based on intensity of sunlight)*
Spectrum of substance: *[e.g. lambda (max.)(>295nm) and epsilon (max) or epsilon (295nm)]*
. . . . . nm
Concentration of Substance: . . . . . .
Temperature: . . . . . °C
Direct photolysis:
Half life: 0.053 days. . . . . .
Degradation: . . . . . % (weight/weight) after . . . . . (exposure time)
Quantum yield: . . . . . .
Indirect Photolysis:
Type of sensitizer: . . . . . .
Concentration of sensitizer: . . . . . .
Rate constant (radical): . . . . . cm^3/molecule*sec
Degradation: . . . . . .
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)]
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity:. . . . . .
Remarks: . .....
Reference: .EPIWIN.....

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life: . . . . . at pH . . . . . at . . . . . °C
Degradation: . . . . . at pH . . . . . at . . . . . °C after
. . . . . (exposure time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: *(e.g. CAS number, name and percentage of degradation products)*
. .....
Reference: . .....

3.1.3 STABILITY IN SOIL

Type : Field trial **[ ]**; Laboratory **[ ]**; Other **[ ]**
Radiolabel: Yes **[ ]** No **[ ]** ? **[ ]**
Concentration: . . . . . .
Soil temperature: . . . . . °C
Soil humidity: . . . . . .
Soil classification: DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[ ]**
year . . . . . .
Content of clay etc.: Clay . . . . . %, Silt . . . . . %, Sand . . . . . %
Organic Carbon: . . . . . .
Soil pH: . . . . . .
Cation exchange capacity: . . . . . .
Microbial biomass: . . . . . .
Dissipation time: DT 50 : . . . . . .
DT 90 : . . . . . .
Dissipation : . . . . . % after . . . . . (time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

*3.2 MONITORING DATA (ENVIRONMENTAL)

Note that data on biological effects monitoring, including biomagnification, and biotransformation and kinetics in environmental species are to be reported in section 4.7 and 4.8, respectively. Nonetheless, concentration in various biota should be reported here. Data on concentration in the workplace or indoor environment should be reported under item 5.11.

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**
Media: . .....
Results: . .....
Remarks: . .....
Reference: . .....

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS *(e.g. during the chemical life-cycle. The information should indicate whether the calculation is on a global basis or is site-specific, and whether it is based on laboratory measurements or field observations.)*

*3.3.1 TRANSPORT

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media: .....
Method: .....
Results: .....
Remarks: .....
Reference: .....

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**;
Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**
Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[x]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**
EPOIWIN. .....
Results: Air 0.0697% to 0.0105%; 1.28hr to 1.26 hr half-life; 1000 kg/hr
Water 17.4% to 1.27%; 900 hr to 3.6e+003 half-life; 1000 kg/hr
Soil 49.6% to 32 %, 900 hr to 3.6e+003 half-life, 1000 kg/hr
Sediment 33% to 66.7%, 3.6e+003 to 1.44e+004 half-life, 0 kg/hr. .....
Remarks: .....
Reference: .EPIWIN.....

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

Results: .....
Remarks: .....
Reference: .....

*3.5 BIODEGRADATION

Type: aerobic **[ ]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[ ]**; .....
Concentration of the chemical: . . . . . related to COD **[ ]**; DOC **[ ]**; test substance **[ ]**
Medium: water **[ ]**; water-sediment **[ ]**; soil **[ ]**; sewage treatment **[ ]**
Degradation: *(percentage reduction/exposure time)*
. . . . . % after . . . . . (time)
Results: *(see OECD Guidelines)* readily biodeg. **[ ]**; inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic (e.g. Zahn-Wellens-Test) . . . . . % in . . . . . (time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: *[In the case of poorly soluble chemicals, treatment given (nature, concentration, CAS number, name and percentage of degradation products etc.)]:*. .....
.....

Reference: .....

3.6 BOD$_5$, COD OR RATIO BOD$_5$/COD

BOD$_5$
Method: . . . . . .
Concentration: . . . . . related to COD **[ ]**; DOC **[ ]**; Test substance **[ ]**
Value: . . . . . mg O_2/l
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

COD
Method: . . . . . .
Value: . . . . . mg O_2/g
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Ratio BOD$_5$/COD: . . . . . .
Remarks: .....
Reference: .....

3.7 BIOACCUMULATION

Species: .....
Exposure period: .....
Temperature: . . . . . °C
Concentration: . . . . . .
BCF: . . . . . .
Elimination: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
.....
Type of test: calculated **[ ]**; measured **[ ]**
static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity:. . . . . .
Remarks: .....
Reference: .....

3.8 ADDITIONAL REMARKS

A. Sewage treatment *(information on treatability of the substance)*

Results: .....
Remarks: .....
Reference: .....

B. Other information *[information that will help to focus the exposure assessment (either qualitative or quantitative)]*

Results: . .....
Remarks: . .....
Reference: . .....

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species: . .....
Exposure period: . .....
Results: LC_{50} (24h) = ... mg/l
LC_{50} (48h) = ... mg/l
LC_{50} (72h) = ... mg/l
LC_{50} (96h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**;
open-system **[ ]**; closed-system **[ ]**
Species: . .....
Exposure period: . .....
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (..h) = ... mg/l
NOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

B. Other aquatic organisms

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Exposure period: . .....
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (..h) = ... mg/l
NOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

***4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae**

Species: . .....
Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[ ]**
Exposure period: . .....
Results: . . . . . EC_{50} (. . . . . .h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . .h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
open-system **[ ]**; closed-system **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.4 TOXICITY TO BACTERIA *(Single species tests and tests on overall processes such as nitrification or soil respiration are included in this item.)*

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: . .....
Exposure Period: . .....
Results: EC_{50} (. . . h) = ... mg/l
EC_{xx} (. . . h) = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used*
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH (*effects on reproduction, embryo/larva, etc.*)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[ ]**
Exposure period: . .....
Results: . . . . . EC_{50} (..d) = ... mg/l
(Endpoint) EC_{xx} (..d) = ... mg/l
NOEC = ...mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

(*)4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES *(e.g. daphnia reproduction. The need to conduct tests for this endpoint will depend <u>inter alia</u> upon possible concern for long term effects.)*

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period: . . . . . .
Results: . . . . . EC_{50} (. . . . . h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . d) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[ ]**
Species: . .....
Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period: .. ..
Results: . . . . . EC_{50} (. . . . . d) = ... mg/kg
(Endpoint) EC_{50} (. . . . . d) = ... mg/kg
EC_{xx} (. . . . . d) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)
Species: . .....
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period: . .....
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

(b)
Species: . .....
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period: . .....
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: . .....

Reference: . .....

(c)

Species: ..... .

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**

Exposure period: . .....

Results: EC_{50} and/or LC_{50} (7d) = ... mg/l

EC_{50} and/or LC_{50}(14d) = ... mg/l

EC_{xx} and/or LC_{xx} (xxd) = ...mg/l

NOEC = ...mg/l

LOEC = ...mg/l

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: . .....

Reference: . .....

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species: . .....

Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[ ]**

Exposure period: . .....

Results: LD_{xx} or LC_{xx} (xxd) = ... mg/kg

NOEC = ... mg/kg

LOEC = ... mg/kg

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:....., purity: .....

Remarks: . .....

Reference: . .....

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

(Studies on variation of predominant species in certain ecosystems (e.g. mesocosm) and monitoring of biological effects are included.)

Results: Substance:.....

Species or ecosystem studied: .....

Effects monitored: .....

Results:.....

Chemical analysis:.....

Remarks: *(Information on environmental conditions (e.g. water characteristics: suspended matter, pH, temperature, hardness; soil/sediment characteristics: % organic matter, clay content)*

.....
Reference: .....

4.8 BIOTRANSFORMATION AND KINETICS

(Under this item, studies on absorption, distribution, metabolism and excretion etc. should be given.)

Type: Animal **[ ]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Results: .....
Remarks: .....
Reference: .....

4.9 ADDITIONAL REMARKS

Results: .....
Remarks: .....
Reference: .....

5. <u>TOXICITY</u>

(Where observations on humans are available, these should be entered in the appropriate "Comments" section or under section 5.11.)

***5.1 ACUTE TOXICITY**

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: . .....
Value: . . . . . mg/kg b.w.:
Discriminating dose: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Exposure time: .....
Value: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Value: . . . . . mg/kg b.w.
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

(e.g. subcutaneous, intravenous, etc.)

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Route of Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time: .....
Value: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain: .....
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: *(If possible, according to EC Directive 67/548/EEC)*
Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[ ]**; Not irritating **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .

Remarks: .....
Reference: .....

5.2.2 EYE IRRITATION/CORROSION

Species/strain: .....
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.3 SKIN SENSITISATION

Type: Magnusson & Kligman Maximazation Test
Species/strain: Guinea Pig/Dunkin Hartley
Results: Sensitizing **[ ]**; Not sensitizing **[x]**; Ambiguous **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Sensitizing **[ ]**; Not sensitizing **[x]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
OECD 406 B6 of EC Directive 92/69/EEC.....
GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance: Good-rite® 3128 (Vanlube® 961) , purity: 99% . . . . . .
Remarks: .....
Reference: Safepharm Laboratories Limited, Project No. 826/015, 01 May 1996, BFGoodrich Co. Sponsor

Reliable (Robust Summary)

*5.4 REPEATED DOSE TOXICITY

Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: .....
Frequency of treatment: .....
Post exposure observation period: .....
Dose: .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL: .....
LOEL: .....
Results: .....

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Reference: . .....

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: *(e.g. Bacterial reverse mutation assay, Bacterial gene mutation study, Cytogenetic Assay etc.)* .....
.....

System of testing: .....

Concentration: .....

Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[ ]**; No data **[ ]**

Results:

Cytotoxicity conc: With metabolic activation: .....
Without metabolic activation: .....

Precipitation conc: .....

Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[ ]**
Without metabolic activation:	**[ ]**	**[ ]**	**[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:....., purity: .....

Remarks: .....

Reference: .....

B. NON-BACTERIAL IN VITRO TEST

Type: *(e.g. mammalian cell gene mutation assay, cytogenetic assay, etc.)*
. .....

System of testing: . .....

Concentration: . .....

Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[ ]**; No data **[ ]**

Results:

Cytotoxicity conc: With metabolic activation:. .....
Without metabolic activation:. .....

Precipitation conc: . .....

Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[ ]**
Without metabolic activation:	**[ ]**	**[ ]**	**[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

* 5.6 GENETIC TOXICITY IN VIVO

Type: *(e.g. micronucleus assay, etc.)*
.....
Species/strain: . .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: . .....
Doses: . .....
Results:
Effect on mitotic
index or P/N ratio: . .....
Genotoxic effects: + ? -
[ ] [ ] [ ]
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

5.7 CARCINOGENICITY

Species/strain: . .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: . .....
Exposure period: . .....
Frequency of treatment: . .....
Postexposure observation period: .....
Doses: . .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results: . .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**; Other **[ ]**
Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:.....
Exposure period: .....
Frequency of treatment: .....
Post exposure observation period: .....
Premating exposure period: male: . . . . . , female: .....
Duration of the test: .....
Doses: .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Parental: .....
NOEL F1 Offspring: .....
NOEL F2 Offspring: .....
Results: .....
General parental toxicity:.....
Toxicity to offspring: *(weights of litter, postnatal growth, viability, etc.)*
.....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: ..... .
Duration of the test: .....
Exposure period: .....
Frequency of treatment: .....
Doses: .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Maternal Toxicity: .....
NOEL teratogenicity : .....
Results: .....
Maternal general toxicity:.....
Pregnancy/litter data:.....
Foetal data: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: *(e.g. neurotoxicity, immunotoxicity, etc.)*
. .....
Results: . .....
Remarks: . .....
Reference: . .....

B. Toxicodynamics, toxicokinetics

Type: *(e.g. toxicodynamics, toxicokinetics)*
. .....
Results: . .....
Remarks: . .....
References: . .....

```
SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
CAS NUM: 015721-78-5
MOL FOR: C28 H43 N1
MOL WT : 393.66
------------------------------ EPI SUMMARY (v3.04) --------------------------
 Physical Property Inputs:
    Water Solubility (mg/L):   ------
    Vapor Pressure (mm Hg) :   ------
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   ------
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   ------

KOWWIN Program (v1.65) Results:
================================

                  Log Kow(version 1.65 estimate): 10.82

SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
MOL FOR: C28 H43 N1
MOL WT : 393.66
-------+-----+---------------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
-------+-----+---------------------------------------------+---------+--------
 Frag  | 10  |  -CH3    [aliphatic carbon]                 | 0.5473  |  5.4730
 Frag  |  2  |  -CH2-   [aliphatic carbon]                 | 0.4911  |  0.9822
 Frag  | 12  |  Aromatic Carbon                            | 0.2940  |  3.5280
 Frag  |  1  |  -N-   [aliphatic N, two aromatic attach]   |-0.4657  | -0.4657
 Frag  |  4  |  -tert Carbon  [3 or more carbon attach]    | 0.2676  |  1.0704
 Const |     |  Equation Constant                          |         |  0.2290
-------+-----+---------------------------------------------+---------+--------
                                                       Log Kow   =  10.8169


MPBPWIN (v1.31) Program Results:
================================
SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
MOL FOR: C28 H43 N1
MOL WT : 393.66
------------------------ SUMMARY MPBPWIN v1.31 --------------------

Boiling Point:  431.62 deg C (Adapted Stein and Brown Method)

Melting Point:  272.38 deg C (Adapted Joback Method)
Melting Point:  138.36 deg C (Gold and Ogle Method)
Mean Melt Pt :  205.37 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  165.16 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
  (Using BP: 431.62 deg C (estimated))
```

```
  (Using MP: 165.16 deg C (estimated))
    VP:  5.5E-009 mm Hg (Antoine Method)
    VP:  5.05E-008 mm Hg (Modified Grain Method)
    VP:  1.2E-007 mm Hg (Mackay Method)
  Selected VP:  5.05E-008 mm Hg (Modified Grain Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group | 10  |  -CH3              |   21.98  |  219.80
 Group |  2  |  -CH2-             |   24.22  |   48.44
 Group |  4  |  >C<               |    4.50  |   18.00
 Group |  1  |  >NH (nonring)     |   45.28  |   45.28
 Group |  8  |  CH (aromatic)     |   28.53  |  228.24
 Group |  4  |  -C (aromatic)     |   30.76  |  123.04
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  880.98
RESULT- corr |  BOILING POINT in deg Kelvin  |  704.78
             |  BOILING POINT in deg C       |  431.62
-------------------------------------------------------

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group | 10  |  -CH3              |   -5.10  |  -51.00
 Group |  2  |  -CH2-             |   11.27  |   22.54
 Group |  4  |  >C<               |   46.43  |  185.72
 Group |  1  |  >NH (nonring)     |   52.66  |   52.66
 Group |  8  |  CH (aromatic)     |    8.13  |   65.04
 Group |  4  |  -C (aromatic)     |   37.02  |  148.08
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  545.54
             |  MELTING POINT in deg C       |  272.38
-------------------------------------------------------



Water Sol from Kow (WSKOW v1.36) Results:
=========================================
SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
MOL FOR: C28 H43 N1
MOL WT : 393.66
---------------------------------- WSKOW v1.36 Results ------------------------
Log Kow  (estimated)  :  10.82
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  10.82

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      --------------------   -----
```

No Applicable Correction Factors

Log Water Solubility (in moles/L) : -11.307
Water Solubility at 25 deg C (mg/L): 1.939e-006

ECOSAR Program (v0.99e) Results:
==========
SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
tyl)phenyl -
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C28 H43 N1
MOL WT : 393.66
Log Kow: 10.82 (KowWin estimate)
Melt Pt:
Wat Sol: 1.765E-006 mg/L (calculated)

ECOSAR v0.99e Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	1.1e-005 *
Neutral Organics	: Fish	96-hr	LC50	1.49e-006
Neutral Organics	: Fish	14-day	LC50	1.1e-005 *
Neutral Organics	: Daphnid	48-hr	LC50	2.94e-006 *
Neutral Organics	: Green Algae	96-hr	EC50	3.06e-006 *
Neutral Organics	: Fish	30-day	ChV	7.97e-007
Neutral Organics	: Daphnid	16-day	EC50	7.16e-006 *
Neutral Organics	: Green Algae	96-hr	ChV	5e-005 *
Neutral Organics	: Fish (SW)	96-hr	LC50	2.44e-005 *
Neutral Organics	: Mysid Shrimp	96-hr	LC50	7.95e-010
Neutral Organics	: Earthworm	14-day	LC50	4.651 *

Note: * = asterick designates: Chemical may not be soluble
enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.04) Program Results:
==========

```
       Bond Est :  6.76E-005 atm-m3/mole
       Group Est:  Incomplete

SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
MOL FOR: C28 H43 N1
MOL WT : 393.66
--------------------------- HENRYWIN v3.04 Results --------------------------
----------+---------------------------------------------+---------+----------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION           | COMMENT |  VALUE
----------+---------------------------------------------+---------+----------
 HYDROGEN |  34  Hydrogen to Carbon (aliphatic) Bonds   |         | -4.0690
 HYDROGEN |   8  Hydrogen to Carbon (aromatic) Bonds    |         | -1.2344
 HYDROGEN |   1  Hydrogen to Nitrogen Bonds             |         |  1.2835
 FRAGMENT |  14  C-C                                    |         |  1.6283
 FRAGMENT |   2  C-Car                                  |         |  0.3239
 FRAGMENT |  12  Car-Car                                |         |  3.1657
 FRAGMENT |   2  Car-N                                  |         |  1.4608
----------+---------------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE   |  TOTAL  |  2.559
----------+---------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 6.76E-005 atm-m3/mole
                                = 2.76E-003 unitless

--------+---------------------------------------------+------------+--------
        |        GROUP CONTRIBUTION DESCRIPTION       |   COMMENT  |  VALUE
--------+---------------------------------------------+------------+--------
        |           2  Car (N)(Car)(Car)              |  ESTIMATE  | -1.00
        |          10  CH3 (X)                        |            | -6.20
        |           2  CH2 (C)(C)                     |            | -0.30
        |           2  C (C)(C)(C)(C)                 |            |  1.42
        |           2  C (C)(C)(C)(Car)               |            |  1.86
        |           8  Car-H (Car)(Car)               |            |  0.88
        |           2  Car (C)(Car)(Car)              |            |  1.40
        |              MISSING Value for:  NH (Car)(Car)
--------+---------------------------------------------+------------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE | INCOMPLETE | -1.94
--------+---------------------------------------------+------------+--------


Henrys LC [VP/WSol estimate using EPI values]:
    HLC:  1.349E-002 atm-m3/mole
    VP:   5.05E-008 mm Hg
    WS:   1.94E-006 mg/L



BIOWIN (v3.67) Program Results:
==============================
SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
MOL FOR: C28 H43 N1
MOL WT : 393.66
--------------------------- BIOWIN v3.67 Results ---------------------------
```

```
    Linear Model Prediction    :  Does Not Biodegrade Fast
    Non-Linear Model Prediction:  Does Not Biodegrade Fast
    Ultimate Biodegradation Timeframe:  Recalcitrant
    Primary  Biodegradation Timeframe:  Weeks-Months

------+-----+---------------------------------------------+---------+---------
 TYPE | NUM |        BIODEG FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag |  4  |  Carbon with 4 single bonds & no hydrogens  | -0.1839 | -0.7357
 Frag |  1  |  Aromatic amine   [-NH2  or  -NH-]          | -0.2338 | -0.2338
 MolWt|  *  |  Molecular Weight Parameter                 |         | -0.1874
 Const|  *  |  Equation Constant                          |         |  0.7475
============+=============================================+=========+=========
   RESULT   |     LINEAR BIODEGRADATION PROBABILITY       |         | -0.4093
============+=============================================+=========+=========

------+-----+---------------------------------------------+---------+---------
 TYPE | NUM |        BIODEG FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag |  4  |  Carbon with 4 single bonds & no hydrogens  | -1.7232 | -6.8928
 Frag |  1  |  Aromatic amine   [-NH2  or  -NH-]          | -1.9070 | -1.9070
 MolWt|  *  |  Molecular Weight Parameter                 |         | -5.5900
============+=============================================+=========+=========
   RESULT   |   NON-LINEAR BIODEGRADATION PROBABILITY     |         |  0.0000
============+=============================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+---------------------------------------------+---------+---------
 TYPE | NUM |        BIODEG FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag |  4  |  Carbon with 4 single bonds & no hydrogens  | -0.2121 | -0.8485
 Frag |  1  |  Aromatic amine   [-NH2  or  -NH-]          | -0.1349 | -0.1349
 MolWt|  *  |  Molecular Weight Parameter                 |         | -0.8699
 Const|  *  |  Equation Constant                          |         |  3.1992
============+=============================================+=========+=========
   RESULT   |   SURVEY MODEL - ULTIMATE BIODEGRADATION    |         |  1.3458
============+=============================================+=========+=========

------+-----+---------------------------------------------+---------+---------
 TYPE | NUM |        BIODEG FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag |  4  |  Carbon with 4 single bonds & no hydrogens  | -0.1534 | -0.6138
 Frag |  1  |  Aromatic amine   [-NH2  or  -NH-]          | -0.1084 | -0.1084
 MolWt|  *  |  Molecular Weight Parameter                 |         | -0.5680
 Const|  *  |  Equation Constant                          |         |  3.8477
============+=============================================+=========+=========
   RESULT   |   SURVEY MODEL - PRIMARY BIODEGRADATION     |         |  2.5576
============+=============================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

```
AOP Program (v1.89) Results:
============================
SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
MOL FOR: C28 H43 N1
MOL WT : 393.66
-------------------- SUMMARY (AOP v1.89): HYDROXYL RADICALS --------------------
Hydrogen Abstraction       =   4.4989 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 200.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant = 204.4989 E-12 cm3/molecule-sec
   HALF-LIFE =     0.052 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     0.628 Hrs
.......................  ** Designates Estimation(s) Using ASSUMED Value(s)
------------------- SUMMARY (AOP v1.89): OZONE REACTION ----------------------

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

Experimental Database:  NO Structure Matches



PCKOC Program (v1.66) Results:
==============================

                   Koc (estimated): 6.28e+006


SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
MOL FOR: C28 H43 N1
MOL WT : 393.66
--------------------------- PCKOCWIN v1.66 Results ---------------------------

         First Order Molecular Connectivity Index  ........... : 13.074
         Non-Corrected Log Koc  ............................ :  7.5751
         Fragment Correction(s):
                  *   Nitrogen to non-fused aromatic ring ...  : -0.7770
         Corrected Log Koc  ................................ :  6.7981

                          Estimated Koc:  6.282e+006



HYDROWIN Program (v1.67) Results:
=================================
SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
```

```
MOL FOR: C28 H43 N1
MOL WT : 393.66
--------------------------- HYDROWIN v1.67 Results ---------------------------

 Currently, this program can NOT estimate a hydrolysis rate constant for
                the type of chemical structure entered!!

 ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
   and Specific Alkyl Halides can be estimated!!  For more information,
    (Click OVERVIEW in Help  or  see the User's Guide)

              *****   CALCULATION NOT PERFORMED   *****



BCF Program (v2.13) Results:
============================
SMILES : N(c(ccc(c1)C(CC(C)(C)C)(C)C)c1)c(ccc(c2)C(CC(C)(C)C)(C)C)c2
CHEM   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramethylbu
         tyl)phenyl -
MOL FOR: C28 H43 N1
MOL WT : 393.66
---------------------------------- Bcfwin v2.12 ----------------------------------
Log Kow  (estimated)  :  10.82
Log Kow (experimental):  not available from database
Log Kow used by BCF estimates:  10.82

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

      Correction(s):                    Value
       No Applicable Correction Factors
       Minimum Log BCF of 0.50 applied when Log Kow > 7

   Estimated Log BCF =  0.500  (BCF = 3.162)



                            Volatization From Water
                            =======================

Chemical Name: Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetrameth
lbutyl)phenyl -

Molecular Weight    :  393.66 g/mole
Water Solubility    :  -----
Vapor Pressure      :  -----
Henry's Law Constant:  6.76E-005 atm-m3/mole  (estimated by Bond SAR Method)

                             RIVER             LAKE
                           ---------         ---------
Water Depth     (meters):   1                 1
Wind Velocity    (m/sec):   5                 0.5
Current Velocity (m/sec):   1                 0.05

      HALF-LIFE (hours) :   19.21             375.9
```

```
      HALF-LIFE (days ) :   0.8004            15.66


STP Fugacity Model:  Predicted Fate in a Wastewater Treatment Facility
========================================================================
PROPERTIES OF: Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetrameth
lbutyl)phenyl -
-------------
Molecular weight (g/mol)                                 393.66
Aqueous solubility (mg/l)                                0
Vapour pressure (Pa)                                     0
                (atm)                                    0
                (mm Hg)                                  0
Henry 's law constant (Atm-m3/mol)                       6.76E-005
Air-water partition coefficient                          0.00276464
Octanol-water partition coefficient (Kow)                6.60693E+010
Log Kow                                                  10.82
Biomass to water partition coefficient                   1.32139E+010
Temperature [deg C]                                      25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
          -Primary tank        0.00     10000.00       10000.00
          -Aeration tank       0.00     10000.00       10000.00
          -Settling tank       0.00     10000.00       10000.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                             g/h               mol/h          percent

Influent                   1.00E+001         2.5E-002        100.00

Primary sludge             5.99E+000         1.5E-002        59.89
Waste sludge               3.34E+000         8.5E-003        33.36
Primary volatilization     1.09E-008         2.8E-011         0.00
Settling volatilization    2.41E-008         6.1E-011         0.00
Aeration off gas           7.59E-008         1.9E-010         0.00

Primary biodegradation     1.75E-002         4.5E-005         0.18
Settling biodegradation    4.26E-003         1.1E-005         0.04
Aeration biodegradation    5.61E-002         1.4E-004         0.56

Final water effluent       5.96E-001         1.5E-003         5.96

Total removal              9.40E+000         2.4E-002        94.04
Total biodegradation       7.79E-002         2.0E-004         0.78


Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N- 4-(1,1,3,3-tetramet
ylbutyl)phenyl -
  Molecular Wt: 393.66
  Henry's LC  : 6.76e-005 atm-m3/mole (Henrywin program)
  Vapor Press : 5.05e-008 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.23e-006 mm Hg  (super-cooled)
  Melting Pt  : 165 deg C (Mpbpwin program)
  Log Kow     : 10.8  (Kowwin program)
  Soil Koc    : 2.71e+010  (calc by model)
```

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0105	1.26	1000
Water	1.27	3.6e+003	1000
Soil	32	3.6e+003	1000
Sediment	66.7	1.44e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	6.23e-013	960	17.4	32	0.58
Water	4.11e-015	40.5	210	1.35	7.01
Soil	7.77e-017	1.02e+003	0	34	0
Sediment	7.29e-015	531	221	17.7	7.36

Persistence Time: 5.52e+003 hr
Reaction Time: 6.49e+003 hr
Advection Time: 3.69e+004 hr
Percent Reacted: 85
Percent Advected: 15

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 1.255
Water: 3600
Soil: 3600
Sediment: 1.44e+004
Biowin estimate: 1.346 (recalcitrant)

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

101-67-7
Benzenamine, 4-octyl-N-(octylphenyl)-

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value: 87-95°C
Decomposition: Yes **[ ]** No **[X]** Ambiguous **[ ]**
Sublimation: Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method: FF83.9-1 Initial and Final Melt Point of Organic Compounds
: GLP: Yes **[X]** No **[ ]** ? **[ ]** **Klimisch 1**
Remarks: Capillary Melt Point. .....
Reference: ASTM D-1519 / Flexsys Standard Physical Methods of Analysis

*2.2 BOILING POINT

Value: 200°C
Pressure: at 0.5 mm Hg
Decomposition: Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method: Not Specified
GLP: Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**
Remarks: .....
Reference: Monsanto Company MSDS Flectol ODP May 1971

†2.3 DENSITY (relative density)

Type: Bulk density **[ ]**; Density **[X]**; Relative Density **[ ]**
Value: 1.015
Temperature: 20 °C
Method: FF97.8-1 Flexsys Standard Method 1997
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Remarks: .....
Reference: Flexsys Standard Physical Methods of Analysis

*2.4 VAPOUR PRESSURE

Value: <0.1 mm Hg
Temperature: Not Specified
Method: calculated **[X]**; measured **[ ]**
Not Specified.
GLP: Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**
Remarks: .....
Reference: Monsanto Company MSDS Flectol ODP May 1971

*2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$

Log Pow: 11.26
Temperature: Not Applicable
Method: calculated **[X]**; measured **[ ]**
SRC LogKow (KowWin) Program, 1995.
GLP: Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**
Remarks:
Reference: Meylan,W.M. and. P.H.Howard, 1995 J. Pharm. Sci. 84: 83-92.

.

*2.6 WATER SOLUBILITY

A. Solubility

Value:	<0.1g/100 ml
Temperature:	21°C
Description:	Miscible **[ ]**; Of very high solubility **[ ]**; Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**; Of low solubility **[ ]**; Of very low solubility **[X]**; Not soluble **[ ]**
Method:	Not Specified
GLP:	Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**
Remarks:	.
Reference:	Hawley,G.G. The Condensed Chemical Dictionary, 1977.313

B. pH Value, pKa Value

pH Value:	. . . . .
Concentration:	. . . . .
Temperature:	. . . . . °C
Method:	
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
pKa value	. . . . . at 25°C
Remarks:	.....
Reference:	.....

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;

Vigorous reaction in preliminary test **[ ]**;

No oxidising properties **[ ]**; Other **[ ]**

Method: .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: .....

Reference: .....

†2.12 OXIDATION: REDUCTION POTENTIAL

Value: . . . . . mV

Method:

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: .....

Reference: .....

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value: . . . . . .

Method:

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: .....

Reference: .....

B. Other data

(e.g. Henry's Law constant, fat solubility, surface tension (of aqueous solution), adsorption/desorption on soil, particle size distribution, etc.)

Results: .....

Remarks: .....

Reference: .....

3. ENVIRONMENTAL FATE AND PATHWAYS

*3.1.1 PHOTODEGRADATION

Type: Air **[ ]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: . . . . . nm
Relative intensity: . . . . . *(based on intensity of sunlight)*
Spectrum of substance: . . . . . nm
Concentration of Substance: . . . . . .
Temperature: . . . . . °C
Direct photolysis:
Half life: . . . . . .
Degradation: . . . . . % (weight/weight) after . . . . . (exposure time)
Quantum yield: . . . . . .
Indirect Photolysis:
Type of sensitizer: . . . . . .
Concentration of sensitizer: . . . . . .
Rate constant (radical): . . . . . cm^3/molecule*sec
Degradation: . . . . . .
Method: calculated **[ ]**; measured **[ ]**

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity:. . . . . .
Remarks: .....
Reference: .....

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life: . . . . . at pH . . . . . at . . . . . °C
Degradation: . . . . . at pH . . . . . at . . . . . °C after
. . . . . (exposure time)
Method: .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: *(e.g. CAS number, name and percentage of degradation products)*
.....
Reference: .....

***3.2 MONITORING DATA (ENVIRONMENTAL)**

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**

Media: .....

Results: .....

Remarks: .....

Reference: .....

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

***3.3.1 TRANSPORT**

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**

Media: .....

Method: .....

Results: .....

Remarks: .....

Reference: .....

***3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)**

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**; Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**

Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[ ]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**

.....

Results: .....

Remarks: .....

Reference: .....

***3.5 BIODEGRADATION**

Type: aerobic **[ ]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[ ]**; .....
Concentration of the chemical: . . . . . related to COD **[ ]**; DOC **[ ]**; test substance **[ ]**
Medium: water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation: *(percentage reduction/exposure time)*
. . . . . % after . . . . . (time)
Results: *(see OECD Guidelines)* readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic Method: (e.g. Zahn-Wellens-Test) . . . . % in . . . . . (time)
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

4. ECOTOXICITY

***4.1 ACUTE/PROLONGED TOXICITY TO FISH**

Type of test: static **[X]**; semi-static **[]**; flow-through **[ ]**; other **[ ]**
open-system **[ ]**; closed-system **[X]**
Species: Bluegill Sunfish (lepomis machrochirus)
Exposure period: 96 hours
Results: LC_{50} (24h) = >1000 mg/l
LC_{50} (48h) = >1000 mg/l
LC_{50} (72h) = >1000 mg/l
LC_{50} (96h) = >1000 mg/l
NOEC = 1000 mg/l
LOEC = Not determined
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians.
EPA Ecological Research Series EPA-660/3-75-009 April 1975
GLP: Yes **[X]** No **[ ]** ? **[ ]** **Klimisch 1**
Test substance: Flectol ODP tan powder Lot# NB03-001 (Monsanto)
purity: >90%
Remarks: Solvent = Acetone, reagent grade. Water quality monitored for dissolved oxygen, pH and temperature. Range-finding study used to determine final test concentrations. Quality test - Challenge with Antimycin A. No mortalities under test conditions.....
Reference: Monsanto AB-83-016 Analytical Biochemistry Laboratories July 27, 1983. .....

ACUTE/PROLONGED TOXICITY TO FISH

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[ ]**; closed-system **[X]**
Species: Rainbow Trout [Salmo gairdneri]
Exposure period: 96 Hours

Results:	LC_{50} (24h) = >1000 mg/l LC_{50} (48h) = >1000 mg/l LC_{50} (72h) = >1000 mg/l LC_{50} (96h) = >1000 mg/l NOEC = 1000 mg/l LOEC = .Not Determined
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA Ecological Research Series EPA-660/3-75-009 April 1975.
GLP:	Yes **[X]** No **[ ]** ? **[ ]** **Klimisch 1**
Test substance:	Flectol ODP tan powder Lot# NB03-001 (Monsanto) Purity: >90%
Remarks:	Solvent = Acetone, reagent grade. Water quality monitored for dissolved oxygen, pH and temperature. Range-finding study used to determine final test concentrations. Quality test - Challenge with Antimycin A. No mortalities under test conditions
Reference:	Monsanto AB-83-017 Analytical Biochemistry Laboratories July 22, 1983. .....

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

***A. Daphnia**

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**;
open-system **[ ]**; closed-system **[X]**

Species: Daphnia magna

Exposure period: 48 hours

Results: EC_{50} (24h) = 13 mg/l
EC_{50} (48h) = 7.7 mg/l
NOEC = 1.8 mg/l

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians.
EPA Ecological Research Series EPA-660/3-75-009 April 1975

GLP: Yes **[X]** No **[ ]** ? **[ ]** **Klimisch 1**

Test substance: Flectol ODP tan powder Lot# NB03-001 (Monsanto)
Purity: >90%

Remarks: Solvent = Acetone, reagent grade. Water quality monitored for dissolved oxygen, pH and temperature. Range-finding study used to determine final test concentrations. Bioassay conducted at 20°C.....

Reference: Monsanto AB-83-018 Analytical Biochemistry Laboratories July18, 1983.....

*4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae

Species: Selenastrum capricornutum.....

Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**

Exposure period: 96 Hours

Results: EC_{50} (96h) = >100 mg/l
(Endpoint) EC50 (96h) = >100 mg/l
NOEC = 100 mg/l
LOEC = Not determined

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**

Method: EPA Selenastrum capricornutum Algal Assay Test 1971.....
open-system **[ ]**; closed-system **[ ]**

GLP: Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**

Test substance: 4,4'-Dioctyldiphenylamine, purity: Not determined

Remarks: In a study to determine the water quality effects of common lubrication additives, concentrations ranging from 1-100 mg/l of the test substance had no effect on algal growth.....

Reference: AMRL-TR-125:457-491
Scherfig, J and Dixon, P.S. Use of Unicellular Algae for Evaluation of Potential Aquatic Contaminants. Aerospace Medical Research Laboratory, 1975

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: Sprague-Dawley Albino Rats
Value: >7940 mg/kg b.w.:
Discriminating dose: 7940 mg/kg
Method: Limit Test – Single Oral Dose
GLP: Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**
Test substance: Flectol OPD tan powder #CP22448 (Monsanto) Purity: >90%
Remarks: Five rats, two males and three females, were fed a single oral dose of the test article in a corn oil vehicle by oral gavage, followed by a 14 day recovery period. All animals survived to sacrifice. Only clinical signs noted were slightly reduced appetite and activity for one to two days. All viscera appeared normal at necropsy.
Reference: Monsanto YO-74-017 Younger Laboratories, March 11, 1974

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Exposure time: .....
Value: .....
Method: .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: New Zealand Albino White Rabbits
Value: >7940 mg/kg b.w.
Method: Defined Lethal Dose .....
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: Flectol OPD tan powder #CP22448 (Monsanto) Purity: >90%
Remarks: The test article was applied as a 40% solution in corn oil to the shaved skin of two groups of male and female rabbits at dose levels of 5010 and 7940 mg/kg/bw for a period of 24 hours, followed by a 14 day recovery period. Clinical signs noted were slightly reduced appetite and activity for one or two days. All animals survived to sacrifice. Necropsy results indicated all viscera appeared normal.....
Reference: Monsanto YO-74-017 Younger Laboratories, March 11, 1974

***5.4 REPEATED DOSE TOXICITY**

Species/strain: .....

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Route of Administration: . .....

Exposure period: .....

Frequency of treatment: .....

Post exposure observation period: . .....

Dose: .....

Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;

Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOEL: .....

LOEL: .....

Results: .....

Method: .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance: . . . . . , purity: . . . . . .

Reference: .....

***5.5 GENETIC TOXICITY IN VITRO**

A. BACTERIAL TEST

Type: Ames Bacterial Reverse Gene Mutation.....

System of testing: Salmonella typhimurium and Saccharomyces cerevisiae.....

Concentration: 0.1, 1.0, 10.0, 100.0 and 500.0 micrograms per plate .....

Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**

Results:

Cytotoxicity conc: With metabolic activation: 500.0
Without metabolic activation: 500.0

Precipitation conc: Not Determined

Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[X]**
Without metabolic activation:	**[ ]**	**[ ]**	**[X]**

Method: Ames Mutagenicity Plate Assay 1975

GLP: Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**

Test substance : Flectol OPD tan solid, Lot#NF08-09 (Monsanto) purity: >90%

Remarks: Salmonella typhimurium strains TA-1535, TA-1537, TA-1538, TA-98 and TA100, and Saccharomyces cerevisiae strain D4 were exposed to concentrations of the test article in DMSO at concentrations up to 500 micrograms per plate. The test article did not demonstrate mutagenic activity in any of the assays conducted, both with and without metabolic activation, and was not considered to be mutagenic under the test conditions.

Reference: Monsanto BIO-76-281 Litton Bionetics, Inc. December 30, 1976

B. NON-BACTERIAL IN VITRO TEST

Type: Sister Chromatid Exchange in Mammalian Cells
System of testing: Chinese Hamster Ovary (CHO) cells
Concentration: Not Determined
Metabolic activation: With **[ ]**; Without **[]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation:. Not Determined
Without metabolic activation:. Not Determined
Precipitation conc: Not Determined
Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[X]**
Without metabolic activation:	**[ ]**	**[ ]**	**[X]**

Method: OECD 479 In vitro Sister Chromatid Exchange Assay In Mammalian Cells (1986)
GLP: Yes **[X]** No **[ ]** ? **[ ]** **Klimisch 1**
Test substance: Octylated Diphenylamine, CAS# 101-67-7 purity: >90%.
Remarks: Octylated Diphenylamine was one of 46 chemicals tested for their ability to induce sister chromatid exchanges (SCE) and chromosomal aberations (AB) in cultured Chinese hamster ovary (CHO) cells using the standard OECD 479 protocol with and without exogenous metabolic activation. The test article did not induce a positive response for SCE and AB with and without metabolic activation.
Reference: Loveday, K.S., Anderson, B.E., Resnick, M.A., Zeiger, E. Chrosome Aberation and Sister Chromatic Exchange Tests in Chinese Hamster Ovary Cells in vitro. V: Results with 46 Chemicals., Environ. Mol. Mutagen. (1990), 16(4), 272-303

Type: Cytogenetic Assay, Mammalian Chromosome Aberation
System of testing: Chinese Hamster Ovary (CHO) and Chinese Hamster Lung (CHL) cells
Concentration: Not Determined
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation:.....
Without metabolic activation:.....
Precipitation conc: .....
Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[X]**
Without metabolic activation:	**[ ]**	**[ ]**	**[X]**

Method: In vitro Mammalian Chromosome Aberation Test (OECD 473)
GLP: Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**
Test substance: Octylated Diphenylamine purity: >90%
Remarks: Octylated diphenylamine was one of 25 chemicals tested for the induction of chromosomal aberations in two cultured mammalian cell systems – CHO and CHL. In tests conducted with the S9 activation mix, octylated diphenylamine was negative in both. In tests conducted without the S9 mix, octylated diphenylamine was also negative in both cell systems.
Reference: Sofuni, T., Matsuoka, A., Sawada, M., Ishidate, J.,Zeiger, E., Shelby, M. Mutation Res.(1990), 241(2), 175-213

*** 5.6 GENETIC TOXICITY IN VIVO**

Type: Mammalian Germ Cell Mutation
Species/strain: Mice and rats
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: Oral gavage
Exposure period: .....
Doses: .....
Results:
Effect on mitotic index or P/N ratio: .....
Genotoxic effects: + ? -
[X] [ ] [ ]
Method: Rat Dominant Lethal Assay and Unscheduled DNA Synthesis
GLP: Yes **[ ]** No **[ ]** ? **[X]** **Klimisch 2**
Test substance: 4,4'-Dioctyldiphenyamine purity: >90%
Remarks: Weak positive evidence of activity of the test article was noted, but the effects were judged to be marginal. The authors concluded that no clear trends showing a significant potential for genetic effects could be established, and that the type of weak positive data obtained did not support the conclusion that the test article represents a serious genetic or carcinogenic risk to mammals.
Reference: Brusnick, D., Matheson, D. Litton Bionetics, Inc. AMRL-TR-78-46, Report (1978)

***5.8 TOXICITY TO REPRODUCTION**

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **]**;
Other **[ ]**

Species/strain: .....

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Route of Administration: .....

Exposure period: .....

Frequency of treatment: .....

Post exposure observation period: .....

Premating exposure period: male: . . . . . , female: .....

Duration of the test: .....

Doses: .....

Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOEL Parental: .....

NOEL F1 Offspring: .....

NOEL F2 Offspring: .....

Results: .....
General parental toxicity: .....
Toxicity to offspring:
.....

Method: .....
.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance: . . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

***5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY**

Species/strain: .....

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Route of Administration: .....

Duration of the test: .....

Exposure period: .....

Frequency of treatment: .....

Doses: .....

Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;

Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOEL Maternal Toxicity: .....

NOEL teratogenicity : .....

Results: .....

Maternal general toxicity: .....

Pregnancy/litter data: .....

Foetal data:.....

Method: .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance: . . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: Teratogenicity

Frog embryos and larvae.....

Results: Several additives commonly found in aviation lubricants were tested for their potential effects as runoff pollutants in surface waters around Air Force bases. Dioctyldiphenylamine in water had no deleterious effects on the development of frog embryos or larvae under the test conditions.

Remarks: .....

Reference: Greenhouse, G.A. (1975) Effects of Pollutants on Embryos and Larvae of Frogs: A System for Evaluating the Teratogenic Effects of Compounds in Freshwater Environments. Aerospace Medical Research Laboratory, Tech Report AMRL-TR-125:493-511

B. Toxicodynamics, toxicokinetics

Type: *(e.g. toxicodynamics, toxicokinetics)*

.....

Results: .....

Remarks: .....

References: .....

*** 5.11 EXPERIENCE WITH HUMAN EXPOSURE**

Results: .
Remarks: .....
Reference: .....

Results: .....
Remarks: .....
Reference: .....

Results: .....
Remarks: .....
Reference: .....

6. REFERENCES

1) Monsanto Company. Toxicology Profile Flectol ODP. Original, November 15, 1988 by J.W. Barnett, Jr. Update November 10, 1992 by C.E. Healy
2) ASTM D-1519 / Flexsys Standard Physical Methods of Analysis
3) Monsanto Company MSDS Flectol ODP May 1971
4) FF97.8-1 Flexsys Standard Method 1997
5) SRC LogKow (KowWin) Program, 1995. Meylan,W.M. and. P.H.Howard, 1995 J. Pharm. Sci. 84: 83-92
6) Hawley,G.G. The Condensed Chemical Dictionary, 1977.313
7) Acute Toxicity of Flectol ODP to Bluegill Sunfish (Lepomis machrochirus) Monsanto AB-83-016 Analytical Biochemistry Laboratories July 27, 1983
8) Acute Toxicity of Flectol ODP to Rainbow Trout (Salmo gairdneri) Monsanto AB-83-017 Analytical Biochemistry Laboratories July 22, 1983
9) Acute Toxicity of Flectol ODP to Daphnia magna Monsanto AB-83-018 Analytical Biochemistry Laboratories July 28, 1983
10) AMRL-TR-125:457-491 Scherfig, J and Dixon, P.S. Use of Unicellular Algae for Evaluation of Potential Aquatic Contaminants. Aerospace Medical Research Laboratory, 1975
11) Acute Oral Toxicity of Flectol ODP to Albino Rats, Monsanto YO-74-017 Younger Laboratories, March 11, 1974
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13) Mutagenicity of Flectol ODP, Monsanto BIO-76-281 Litton Bionetics, Inc. December 30, 19761814) Loveday, K.S., Anderson, B.E., Resnick, M.A., Zeiger, E. Chrosome Aberation and Sister Chromatic Exchange Tests in Chinese Hamster Ovary Cells in vitro. V: Results with 46 Chemicals., Environ. Mol. Mutagen. (1990), 16(4), 272-303
15) A Comparison of Chromosome Aberation Induction by 25 Compounds Tested by Two Chinese Hamster Cell (CHL and CHO) Systems in Culture. Sofuni, T., Matsuoka, A., Sawada, M., Ishidate, J.,Zeiger, E., Shelby, M. Mutation Res.(1990), 241(2), 175-213
16) Mutagen and Oncogen Study on 4,4-Dioctyldiphenylamine, Brusnick, D., Matheson, D. Litton Bionetics, Inc. AMRL-TR-78-46, Report (1978)
17) Greenhouse, G.A. (1975) Effects of Pollutants on Embryos and Larvae of Frogs: A System for Evaluating the Teratogenic Effects of Compounds in Freshwater

Environments. Aerospace Medical Research Laboratory, Tech Report AMRL-TR-125:493-511

I U C L I D

D a t a S e t

Existing Chemical	ID: 36878-20-3
CAS No.	36878-20-3
EINECS Name	bis(nonylphenyl)amine
EINECS No.	253-249-4
Molecular Formula	C30H47N

Producer Related Part	
Company:	Epona Associates, LLC
Creation date:	11-APR-2001
Substance Related Part	
Company:	Epona Associates, LLC
Creation date:	11-APR-2001

Printing date:	02-NOV-2001
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Reliability (profile):	Reliability: 1, 2
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 Melting Point
-

2.2 Boiling Point
-

2.4 Vapour Pressure
-

2.5 Partition Coefficient
-

2.6.1 Water Solubility
-

3.1.1 Photodegradation
-

3.1.2 Stability in Water
-

3.3.1 Transport between Environmental Compartments
-

3.5 Biodegradation

Type:	aerobic
Inoculum:	activated sludge
Concentration:	100 mg/l related to Test substance
Contact time:	28 day
Degradation:	= 8 % after 28 day
Result:	under test conditions no biodegradation observed
Controlsubstance:	Benzoic acid, sodium salt

Deg. Product: no
Method: OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year: 1997 GLP: yes
Test substance: other TS
Remark: Control substance: >60% in 3 days
Innoculum: Return activated sludge from domestic wastewater treatment plant.
Result: The test substance showed a low biodegradation rate (8.0%) in 28 days. The reference substance, sodium benzoate, reached a level of 82.3% in the same test period.
Test conditions:Inoculum: The supernatant from the homogenized activated sludge was used as inoculum. The inoculum was pre-adapted to the test material for 14 days during which the test substance was added incrementally at concentrations equivalent to 4, 4 and 8 mg carbon/L on days 0, 7, and 12, respectively. The targeted microbial level in the test mixture was 10,000 to 1,000,000 cells/mL. Concentration of test chemical: Test substance concentration was approximately 100 mg/L mineral medium, giving at least 50 to 100 mg ThOD per L medium.
No organic solvents were used to facilitate the dispersion of the test material. The test substance was weighed onto a teflon coupon and introduced into the medium. Temp of incubation: 23 ± 1ºC. Dosing procedure: A measured volume of the inoculated mineral medium containing approximately 100 mg/L test substance is continuously stirred in a closed system for 28 days.
Sampling frequency: The oxygen uptake were monitored continuously and recorded every 4 hours throughout the test.
Controls: Yes (blank and positive controls per guideline); abiotic and toxicity checks were not included. Sodium benzoate was used as the positive control. Analytical method: Oxygen uptake was measured using a BI-1000 electrolytic respirometer system. Method of calculating measured concentrations: N/A.
Other: The inoculum was pre-adapted to the

test substance for 14 days.
Test substance: Benzamine, ar-nonyl-N-(nonylphenyl)-
Reliability: (1) valid without restriction
02-NOV-2001 (1)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: semistatic
Species: *Pimephales promelas* (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: c > 10000
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1993 GLP: yes
Test substance: other TS
Remark: Statistical methods were not used as there were no deaths at the highest test concentration.
Test conditions: Test Organisms: Source - Aquatic Research Organisms, Hampton, New Hampshire; Age- Juvenile; Length - not determined; Wet weight - 0.41 g; Loading rate - 0.27 g/L; Pretreatment - none, fish were acclimated to the test conditions for 14 days prior to start of test. Test System: The static acute screening test was conducted using nominal test concentrations of 1,000 mg/L, 5,000 mg/L and 10,000 mg/L. The test substance was directly added to the dilution water and no solvent was used. The test was conducted in 20 L, polyethylene-lined, glass aquaria that contained 15 L of test solution. 10 fish were used for each test concentration (no replicates were used). Test media was renewed after 48 hours. The fish were not fed during the test. Dilution Water: Source - Dechlorinated tap water; Hardness - Water adjusted to a hardness of 172 - 176 mg/L as $CaCO_3$; Analysis - Water was free of measurable quantities of pesticides; Water chemistry in test: DO (% Saturation) - 92 to 104%; pH - 7.2 to 8.0Test Temperature (°C) - 22 ± 1Test Levels: Control, 1,000, 5,000 and 10,000 mg/L
Test method: U.S. EPA TSCA 797.1400 (1985)
Test substance: Benzamine, ar-nonyl-N-(nonylphenyl)-
Remark: A sheen of insoluble material was observed in all non-control test vessels.
Reliability: (1) valid without restriction
02-NOV-2001 (4)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: semistatic
Species: *Mysidopsis bahia* (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: c = 250
EC50: c = 733
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute

Immobilisation Test"
Year: 1991 GLP: yes
Test substance:
Method: Test method: Static renewal with WAF
Remark: EL50's were calculated using standard statistical methods from Stephan (1983). Results: Effect concentrations based on nominal loading rates. Control response was satisfactory (>90% survival and no sublethal effects).
Results: Mysids exposed to 600 mg/L were lethargic and exhibited erratic swimming from 48 to 96 hours. No other sublethal effects were observed in any test vessel during the 96 hour exposure.
Test conditions: Test species: Juvenile mysids less than 24-hours old were produced from laboratory in-house culture. Test System: The test was conducted using the water accommodated fraction (WAF) of nominal test concentrations. Individual WAFs were prepared by adding a measured weight of test material to a measured volume of dilution water (1-L) in a glass vessel and stirring for 24 hours. Following the mixing period, the test solutions were allowed to stand for 1 hour before the water phase was siphoned off. The siphoned water phase (i.e., WAF) was used for the aquatic toxicity test.Test conditions: A 2-L glass beaker that contained 1 L of test solution was used per treatment. The test vessels were loosely covered to reduce entry of dust, etc. Mysids were fed newly hatched *Artemia salina nauplii* once or twice daily during the test. Dilution water: Seawater collected from the Atlantic Ocean in Hampton, New Hampshire was used. Water was adjusted to a salinity of 20 parts per thousand and aerated. Water was free of pesticides and PCBs at the detection limit. Water chemistry; pH - 8.1; TOC - 3.9 to 8.2. Element: Immobilization/mortality. Test Temperature (ºC) - 24 ± 1. Test Levels: Control, 150, 250, 400, 600 and 1,000 mg/L nominal test concentrations. The WAF was used for testing. 10 mysids per test vessel (2 replicates per test concentration were used).
Test method: US EPA TSCA #797.1300 (1985)
Reliability: (1) valid without restriction
02-NOV-2001 (2)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: *Selenastrum capricornutum* (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: c = 33
EL50 : c = 600
EL0 : c = 870

Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1997 GLP: yes
Test substance: other TS
Remark: Effects were determined to be algistatic based on the rapid re-growth of an aliquot of cells taken from 500 mg/L cultured in fresh control media.
EL50s were calculated using Standard statistical methods from Stephan (1983)
Method: US EPA TSCA, 797.1050
Test conditions: Test Species: Cells taken from a log-growth phase in-house culture of *Selenastrum capricornutum* that was originally purchased from University of Texas at Austin alga collection. Test System: Individual WAFs were prepared for each test level and renewed daily. Individual WAFs were prepared by adding a measured weight of test material to a measured volume of dilution water (1-L) in a glass vessel and stirring for 24 hours. Following the mixing period, the test solutions were allowed to stand for approximately 4 hours before the water phase was siphoned off. The siphoned water phase (i.e., WAF)was used for the aquatic toxicity test. Test Conditions: A static test was conducted; i.e., there was no daily renewal of test solution. Three 100-mL replicates per treatment, inoculum ~10,000 cells/mL. The 250-mL Erlenmeyer flasks were stoppered with foam plugs to reduce entry of dust, etc. During the test all treatment and control flasks were randomly placed on an orbital shaker adjusted to approximately 100 cycles per minute under constant light (24 hours/day). Daily cell counts were made visually by means of direct microscopic examination with a hemocytometer. Light: Cool-white fluorescent lights provided a light intensity of 370 to 380 foot-candles 24-h per day. Test temperature (°C) - 24 ± 1. Dilution Water: Sterile enriched alga growth media adjusted to pH 7.5. Particulate matter ranged from <10 mg/L at the start of the test to 29 mg/L at the end of the test. pH ranged from 7.6 - 8.1 at 0-hour and 9.0 - 9.7 after 96 hours. Test Levels:
Control, 0.3, 3.3, 33, 330 and 3,300 mg/L WAF loading rates.
Test substance: Benzamine, ar-nonyl-N-(nonylphenyl)-
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
02-NOV-2001 (3)

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity
-

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity
-

5.1.4 Acute Toxicity, other Routes
-

5.4 Repeated Dose Toxicity
-

5.5 Genetic Toxicity 'in Vitro'
-

5.6 Genetic Toxicity 'in Vivo'
-

5.8 Toxicity to Reproduction
-

5.9 Developmental Toxicity/Teratogenicity
-

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(3) Acute toxicity of the water accommodated fraction (WAF) of benzenamine, ar-nonyl-N-(nonylphenyl)- to the freshwater algae Selenastrum capricornutum. Wilbury Labs, 11 Sept 1997.

(4) Acute toxicity of benzenamine, ar-nonyl-N-(nonylphenyl)- to the fathead minnow, Pimephales promelas. Wilbury Labs, 15 Jan 1993.

96-h EL50s = 200 mg/L (biomass), 96-h EL0s 220 mg/L (biomass)

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE . . . . . CHEMICAL

Benzenamine, 2-ethyl-N-(2-ethyl[phenyl)-, (tripropenyl) derivatives. . . . . .

CAS No. 68608-77-5

Sponsor Country : . . . . . .

DATE: . . . . . .

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. Cast number** 68608-77-5

B. Name *(IUPAC name)* .....

***C. Name** *(OECD name)* .....

†D. CAS Descriptor *(where applicable for complex chemicals)*

Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives

E. EINECS-Number 271-800-7

F. Molecular Formula .....

***G. Structural Formula** *(indicate the structural formula in smiles code, if available)*

.....

H. Substance Group *(if possible, only for petroleum products, see HEDSET explanatory note)*

.....

I. Substance Remark *(Indicate the substance remark as prescribed in the EINECS Inventory, if possible)*

.....

J. Molecular Weight 225-479 .....

1.02 OECD INFORMATION

A. Sponsor Country: United States.....

B. Lead Organisation:

Name of Lead Organisation:
American Chemistry Council, Rubber and Plastic Additives (RAPA) HPV Panel

Street: 1300 Wilson Boulevard
Town: VA 22209 Arlington
Country: United States
Phone: 703-741-5600
Fax: 703-741-6091

C. **Name of responder** *(Information on a responder should be provided when companies respond to Lead Organisation or SIDS Contact Points.)*

Name: .....
Address: .....
Street: .....
Postal code: .....
Town: .....
Country: .....
Tel: .....
Fax: .....

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [x]; organometallic [ ];
petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [x]; solid **[ ]**

C. Purity *(indicate the percentage by weight/weight) 100 %* .....

1.2 SYNONYMS Good-rite® NEPA; Vanlube® NA; Goodrite® 3185
.....
.....

1.3 IMPURITIES *[Indicate CAS No., chemical name (IUPAC name is preferable), percentage, if possible EINECS number.]*

CAS No: . . . . . - . . . . . - . . . . . .
EINECS No: .....
Name: .....
Value: .....
Remarks: .....

1.4 ADDITIVES *(e.g. stabilising agents, inhibitors etc. Indicate CAS No., chemical name (IUPAC name is preferable), percentage, if possible EINECS number), the component of the UVCB (substance with no defined composition) should be indicated here.*)

CAS No: . . . . . - . . . . . - . . . . . .
EINECS No: . . . . . - . . . . . - . . . . . .
Name: .....
Value: .....
Remarks: .....

2. PHYSICAL-CHEMICAL DATA

***2.1 MELTING POINT** *(If more than one, identify the recommended value.)*

Value: . . . . . .°C
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updated of the method used)]*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

***2.2 BOILING POINT** *(If more than one, identify the recommended value.)*

Value: 443.18 – 547.61 °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Based on the two reaction products that are 90+% of all reaction products..
Reference: EPIWIN.....

†2.3 DENSITY (relative density) *(Where applicable, indicate the relative density of the substance.)*

Type: Bulk density **[ ]**; Density **[ ]**; Relative Density **[ ] Specific Gravity**
Value: 0.915-0.955
Temperature: . . . . . °C
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: BFGoodrich MSDS.....

***2.4 VAPOUR PRESSURE** *(if more than one, identify the recommended value)*

Value: 2.35E-008 to 9.18E-012 hPa
Temperature: 25 °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updated of the method used)].
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Based on the two reaction products that are 90+% of all reaction products.
Reference: EPIWIN.....

***2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$** *(if more than one, identify the recommended value)*

Log Pow: 9.84. . . . . .
Temperature: . . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)].
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Based on the two reaction products that are 90+% of all reaction products.
Reference: EPIWIN.....

***2.6 WATER SOLUBILITY** *(if more than one, identify the recommended value)*

A. Solubility

Value: 2.35e-005 to 5.85e-010
Temperature: 25 °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Based on the two reaction products that are 90+% of all reaction products.
Reference: EPIWIN .....

Solubility

Value: . **Insoluble** . . . . . .
Temperature: ……. °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: BFGoodrich MSDS.....

B. pH Value, pKa Value

pH Value: . . . . . .
Concentration: . . . . . .
Temperature: . . . . . °C
Method: *[e.g. OECD, other (with the year of publication or updating of the method used).*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
(Where applicable, enter values for the dissociation constant(s) and the conditions under which they were measured.)
pKa value . . . . . at 25°C
Remarks: . .....
Reference: . .....

2.7 FLASH POINT *(liquids)*

Value: 213 °C
Type of test: Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**
Method: *(with the year of publication or updating of the method used).* .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.8 AUTO FLAMMABILITY *(solid/gases)*

Value: . . . . . °C
Pressure: . . . . . hPa
Method: *(with the year of publication or updating of the method used).* .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.9 FLAMMABILITY

Results: Extremely flammable **[ ]**; Extremely flammable - liquified gas **[ ]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method: *(with the year of publication or updating of the method used).* .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.10 EXPLOSIVE PROPERTIES

Results: Explosive under influence of a flame**[ ]**;

More sensitive to friction than m-dinitrobenzene **[ ]**;
More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**;
Other **[ ]**

Method: *(with the year of publication or updating of the method used)*. .....
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: . .....

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;
Vigorous reaction in preliminary test **[ ]**;
No oxidising properties **[ ]**; Other **[ ]**

Method: *(with the year of publication or updating of the method used)*. .....
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: . .....

†2.12 OXIDATION: REDUCTION POTENTIAL

(Where applicable, indicate the redox potential and the conditions under which it was measured.)

Value: . . . . . mV

Method: *(with the year of publication or updating of the method used)*
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: . .....

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value: . . . . . .

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: . .....

B. Other data

(e.g. Henry's Law constant, fat solubility, surface tension (of aqueous solution), adsorption/desorption on soil, particle size distribution, etc.)

Results: . .....

Remarks: . .....

Reference: . .....

3. ENVIRONMENTAL FATE AND PATHWAYS

[Reporting of studies should give the test method, test conditions (laboratory versus field studies), test results (e.g. % degradation in specified time period) and reference. Information on breakdown products (transient and stable) should be provided when available.]

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air **[x]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: . . . . . nm
Relative intensity: . . . . . *(based on intensity of sunlight)*
Spectrum of substance: *[e.g. lambda (max.)(>295nm) and epsilon (max) or epsilon (295nm)]*
. . . . . nm
Concentration of Substance: . . . . . .
Temperature: . . . . . °C
Direct photolysis:
Half life: 0.05 days to 0.048 days. . . . . .
Degradation: . . . . . % (weight/weight) after . . . . . (exposure time)
Quantum yield: . . . . . .
Indirect Photolysis:
Type of sensitizer: . . . . . .
Concentration of sensitizer: . . . . . .
Rate constant (radical): . . . . . cm^3/molecule*sec
Degradation: . . . . . .
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)]
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity:. . . . . .
Remarks: Based on the two reaction products that are 90+% of all reaction products.
Reference: EPIWIN.....

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life: . . . . . at pH . . . . . at . . . . . °C
Degradation: . . . . . at pH . . . . . at . . . . . °C after
. . . . . (exposure time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: *(e.g. CAS number, name and percentage of degradation products)*
.....
Reference: .....

3.1.3 STABILITY IN SOIL

Type : Field trial **[ ]**; Laboratory **[ ]**; Other **[ ]**
Radiolabel: Yes **[ ]** No **[ ]** ? **[ ]**
Concentration: . . . . . .
Soil temperature: . . . . . °C
Soil humidity: . . . . . .
Soil classification: DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[ ]**
year . . . . . .
Content of clay etc.: Clay . . . . . %, Silt . . . . . %, Sand . . . . . %
Organic Carbon: . . . . . .
Soil pH: . . . . . .
Cation exchange capacity: . . . . . .
Microbial biomass: . . . . . .
Dissipation time: DT 50 : . . . . . .
DT 90 : . . . . . .
Dissipation : . . . . . % after . . . . . (time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

*3.2 MONITORING DATA (ENVIRONMENTAL)

Note that data on biological effects monitoring, including biomagnification, and biotransformation and kinetics in environmental species are to be reported in section 4.7 and 4.8, respectively. Nonetheless, concentration in various biota should be reported here. Data on concentration in the workplace or indoor environment should be reported under item 5.11.

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**
Media: . .....
Results: . .....
Remarks: . .....
Reference: . .....

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS *(e.g. during the chemical life-cycle. The information should indicate whether the calculation is on a global basis or is site-specific, and whether it is based on laboratory measurements or field observations.)*

*3.3.1 TRANSPORT

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media: .....
Method: .....
Results: .....
Remarks: .....
Reference: .....

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**;
Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**
Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[x]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**
EPIWIN.....
Results: Air 0.0424-0.0393%, 1.2-1.15 half-life, 1000 kg/hr emissions
Water 4.34-4.31%, 1.48e+003 half-life, 1000 kg/hr emissions
Soil 56.1-56.4%, 1.48e+003 half-life, 1000 kg/hr emission
Sediment 39.5-39.2%, 1.48e+003 half-life, 1000 kg/hr emission
Remarks: Based on the two reaction products that are 90+% of all reaction products.
Reference: .EPIWIN.....

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

Results: .....
Remarks: .....
Reference: .....

*3.5 BIODEGRADATION

Type: aerobic **[ ]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[ ]**; .....
Concentration of the chemical: . . . . . related to COD **[ ]**; DOC **[ ]**; test substance **[ ]**
Medium: water **[ ]**; water-sediment **[ ]**; soil **[ ]**; sewage treatment **[ ]**
Degradation: *(percentage reduction/exposure time)*
. . . . . % after . . . . . (time)
Results: *(see OECD Guidelines)* readily biodeg. **[ ]**; inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic (e.g. Zahn-Wellens-Test) . . . . . % in . . . . . (time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: *[In the case of poorly soluble chemicals, treatment given (nature, concentration, CAS number, name and percentage of degradation products etc.)]:*.....
.....

Reference: . .....

3.6 BOD$_5$, COD OR RATIO BOD$_5$/COD

BOD$_5$
Method: . . . . . .
Concentration: . . . . . related to COD **[ ]**; DOC **[ ]**; Test substance **[ ]**
Value: . . . . . mg O_2/l
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

COD
Method: . . . . . .
Value: . . . . . mg O_2/g
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Ratio BOD$_5$/COD: . . . . . .
Remarks: . .....
Reference: . .....

3.7 BIOACCUMULATION

Species: . .....
Exposure period: . .....
Temperature: . . . . . °C
Concentration: . . . . . .
BCF: . . . . . .
Elimination: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
Type of test: calculated **[ ]**; measured **[ ]**
static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity:. . . . . .
Remarks: . .....
Reference: . .....

3.8 ADDITIONAL REMARKS

A. Sewage treatment *(information on treatability of the substance)*

Results: . .....
Remarks: . .....
Reference: . .....

B. Other information *[information that will help to focus the exposure assessment (either qualitative or quantitative)]*

Results: .....
Remarks: .....
Reference: .....

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species: .....
Exposure period: .....
Results: LC_{50} (24h) = ... mg/l
LC_{50} (48h) = ... mg/l
LC_{50} (72h) = ... mg/l
LC_{50} (96h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**;
open-system **[ ]**; closed-system **[ ]**
Species: .....
Exposure period: .....
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (..h) = ... mg/l
NOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

B. Other aquatic organisms

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Exposure period: . .....
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (..h) = ... mg/l
NOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

***4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae**

Species: . .....
Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[ ]**
Exposure period: . .....
Results: . . . . . EC_{50} (. . . . . .h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . .h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
open-system **[ ]**; closed-system **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.4 TOXICITY TO BACTERIA *(Single species tests and tests on overall processes such as nitrification or soil respiration are included in this item.)*

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: . .....
Exposure Period: . .....
Results: EC_{50} (. . . h) = ... mg/l
EC_{xx} (. . . h) = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used*
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH (*effects on reproduction, embryo/larva, etc.*)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[ ]**
Exposure period: . .....
Results: . . . . . EC_{50} (..d) = ... mg/l
(Endpoint) EC_{xx} (..d) = ... mg/l
NOEC = ...mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

(*)4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES *(e.g. daphnia reproduction. The need to conduct tests for this endpoint will depend <u>inter alia</u> upon possible concern for long term effects.)*

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period: . . . . . .
Results: . . . . . EC_{50} (. . . . . h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . d) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[ ]**
Species: . .....
Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period: .. ..
Results: . . . . . EC_{50} (. . . . . d) = ... mg/kg
(Endpoint) EC_{50} (. . . . . d) = ... mg/kg
EC_{xx} (. . . . . d) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)
Species: . .....
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period: . .....
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

(b)
Species: . .....
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period: . .....
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: . .....

Reference: . .....

(c)

Species: ..... .

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**

Exposure period: . .....

Results: EC_{50} and/or LC_{50} (7d) = ... mg/l

EC_{50} and/or LC_{50}(14d) = ... mg/l

EC_{xx} and/or LC_{xx} (xxd) = ...mg/l

NOEC = ...mg/l

LOEC = ...mg/l

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: . .....

Reference: . .....

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species: . .....

Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[ ]**

Exposure period: . .....

Results: LD_{xx} or LC_{xx} (xxd) = ... mg/kg

NOEC = ... mg/kg

LOEC = ... mg/kg

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:....., purity: .....

Remarks: . .....

Reference: . .....

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

(Studies on variation of predominant species in certain ecosystems (e.g. mesocosm) and monitoring of biological effects are included.)

Results: Substance:.....

Species or ecosystem studied: .....

Effects monitored: .....

Results:.....

Chemical analysis:.....

Remarks: *(Information on environmental conditions (e.g. water characteristics: suspended matter, pH, temperature, hardness; soil/sediment characteristics: % organic matter, clay content)*

.....
Reference: .....

4.8 BIOTRANSFORMATION AND KINETICS

(Under this item, studies on absorption, distribution, metabolism and excretion etc. should be given.)

Type: Animal **[ ]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Results: .....
Remarks: .....
Reference: .....

4.9 ADDITIONAL REMARKS

Results: .....
Remarks: .....
Reference: .....

5. TOXICITY

(Where observations on humans are available, these should be entered in the appropriate "Comments" section or under section 5.11.)

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[x]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: Rat/Charles River strain (COBS).....
Value: >34,600. . . . . mg/kg b.w.:
Discriminating dose: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[** x **]** ? **[ ]**
Test substance:), Goodrite® 3185. . . . . , purity: 100%. . . . . .
Remarks: .....
Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor .....

Not Reliable

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} [**]**; LCL_0 **[ ]**; Other **[x]**
Species/strain: Rats/Sprague-Dawley.....
Exposure time: 4 hrs.....
Value: (see remarks).....

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[x]** ? **[ ]**

Test substance:.), Goodrite® 3185 . . . . . , purity: 100%. . . . . .

Remarks: No deaths; concentration not measured due to low volatility .....

Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor .....

Not Reliable

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: Rabbit/New Zealand.....

Value: >3,000. . . . . mg/kg b.w.

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[** x **]** ? **[ ]**

Test substance:. Goodrite® 3185 . . . . . , purity: 100%. . . . . .

Remarks: .....

Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor .....

Not Reliable

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION
(e.g. subcutaneous, intravenous, etc.)

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Route of Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time: .....
Value: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain: .....
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: *(If possible, according to EC Directive 67/548/EEC)*
Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[ ]**; Not irritating **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.2.2 EYE IRRITATION/CORROSION

Species/strain: Rabbit/New Zealand.....
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[x]**;
Not irritating **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[** x **]** ? **[ ]**
Test substance:. Goodrite® 3185. . . . . , purity: 100% . . . . . .
Remarks: .....
Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor. .....

Not Reliable

5.3 SKIN SENSITISATION

Type: . .....
Species/strain: . .....
Results: Sensitizing **[ ]**; Not sensitizing **[ ]**; Ambiguous **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Sensitizing **[ ]**; Not sensitizing **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

*5.4 REPEATED DOSE TOXICITY

Species/strain: . .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: . .....
Frequency of treatment: . .....
Post exposure observation period: .....
Dose: . .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL: . .....
LOEL: . .....
Results: . .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Reference: . .....

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: *Bacterial reverse mutation assay*

System of testing: *Salmonella typhimurium,* strains TA-1535, TA-1537, TA-98, TA-100 and .....
Escherichia coli, strain WP2uvrA-.
Concentration: 0, 50, 150, 1500, 5000 ug/plate .....
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[x]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: None toxic
Without metabolic activation: None toxic
Precipitation conc: 1500 and 5000 ug/plate
Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[-]**
Without metabolic activation:	**[ ]**	**[ ]**	**[-]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
OECD B14 in EC Directive 92/69/EEC
GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance: Vanlube NA, purity: ..100 %
Remarks: .....
Reference: Safepharm Laboratories Project No. 860/026, 21 May 1997, Sponsor R.T. Vanderbilt Co., Inc.

Reliable (Robust Summary)

B. NON-BACTERIAL IN VITRO TEST

Type: *(e.g. mammalian cell gene mutation assay, cytogenetic assay, etc.)*
. .....
System of testing: . .....
Concentration: . .....
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[ ]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation:. .....
Without metabolic activation:. .....
Precipitation conc: . .....
Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[ ]**
Without metabolic activation:	**[ ]**	**[ ]**	**[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

* 5.6 GENETIC TOXICITY IN VIVO

Type: *(e.g. micronucleus assay, etc.)*
.....
Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: .....
Doses: .....
Results:
Effect on mitotic index or P/N ratio: .....
Genotoxic effects: + ? -
[ ] [ ] [ ]
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.7 CARCINOGENICITY

Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: .....
Frequency of treatment: .....
Postexposure observation period: .....
Doses: .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**; Other **[ ]**

Species/strain: .....

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Route of Administration:.....

Exposure period: .....

Frequency of treatment: .....

Post exposure observation period: .....

Premating exposure period: male: . . . . . , female: .....

Duration of the test: .....

Doses: .....

Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;

Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOEL Parental: .....

NOEL F1 Offspring: .....

NOEL F2 Offspring: .....

Results: .....

General parental toxicity:.....

Toxicity to offspring: *(weights of litter, postnatal growth, viability, etc.)*

.....

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....

.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species/strain: . .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: ..... .
Duration of the test: . .....
Exposure period: . .....
Frequency of treatment: . .....
Doses: . .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Maternal Toxicity: . .....
NOEL teratogenicity : . .....
Results: . .....
Maternal general toxicity: .....
Pregnancy/litter data: .....
Foetal data: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: *(e.g. neurotoxicity, immunotoxicity, etc.)*
. .....
Results: . .....
Remarks: . .....
Reference: . .....

B. Toxicodynamics, toxicokinetics

Type: *(e.g. toxicodynamics, toxicokinetics)*
. .....
Results: . .....
Remarks: . .....
References: . .....

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE . . . . . CHEMICAL

Benzenamine, N-phenyl-, reaction products with styrene and 2, 4, 4-trimethylpentene

CAS No. 68921-45-9

Sponsor Country : . . . . . .

DATE: . . . . . .

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. Cast number** 68921-45-9

B. Name *(IUPAC name)* .....

***C. Name** *(OECD name)* .....

†D. CAS Descriptor *(where applicable for complex chemicals)*
Benzenamine, N-phenyl-, reaction products with styrene and 2, 4, 4-trimethylpentene

E. EINECS-Number 272-940-1

F. Molecular Formula .....

***G. Structural Formula** *(indicate the structural formula in smiles code, if available)*

.....

H. Substance Group *(if possible, only for petroleum products, see HEDSET explanatory note)*

.....

I. Substance Remark *(Indicate the substance remark as prescribed in the EINECS Inventory, if possible)*

.....

J. Molecular Weight 225-633 .....

1.02 OECD INFORMATION

A. Sponsor Country: United States

B. Lead Organisation:

Name of Lead Organisation:
American Chemistry Council, Rubber and Plastic Additives (RAPA) HPV Panel

Street: 1300 Wilson Boulevard
Town: VA 22209 Arlington
Country: United States
Phone: 703-741-5600
Fax: 703-741-6091

C. **Name of responder** *(Information on a responder should be provided when companies respond to Lead Organisation or SIDS Contact Points.)*

Name: .....
Address: .....
Street: .....
Postal code: .....
Town: .....
Country: .....
Tel: .....
Fax: .....

1.1 GENERAL SUBSTANCE INFORMATION

A. **Type of Substance**

element [ ]; inorganic [ ]; natural substance [ ]; organic [x]; organometallic [ ]; petroleum product [ ]

B. **Physical State** *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [x]; solid **[ ]**

C. **Purity** *(indicate the percentage by weight/weight) 98%*

1.2 **SYNONYMS** Good-rite® 3190NT; Vanlube® SL; Vanlube® SL-HP .....
.....
.....
.....
.....

1.3 **IMPURITIES** *[Indicate CAS No., chemical name (IUPAC name is preferable), percentage, if possible EINECS number.]*

CAS No: 122-39-4
EINECS No: .....
Name: Diphenylamine .....
Value: <2% .....
Remarks: .....

CAS No: 100-42-5
EINECS No: .....
Name: Styrene .....
Value: <0.0003% .....
Remarks: .....

1.4 **ADDITIVES** *(e.g. stabilising agents, inhibitors etc. Indicate CAS No., chemical name (IUPAC name is preferable), percentage, if possible EINECS number), the component of the UVCB (substance with no defined composition) should be indicated here.*)

CAS No: . . . . . - . . . . . - . . . . . .
EINECS No: . . . . . - . . . . . - . . . . . .
Name: .....
Value: .....
Remarks: .....

2. PHYSICAL-CHEMICAL DATA

***2.1** **MELTING POINT** *(If more than one, identify the recommended value.)*

Value: . . . . . .°C
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updated of the method used)]*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

***2.2** **BOILING POINT** *(If more than one, identify the recommended value.)*

Value: >198 °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: . .....
Reference: BFGoodrich MSDS. .....

BOILING POINT *(If more than one, identify the recommended value.)*

Value: 392.71 TO 663.07 °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: .Range for the components. .....
Reference: EPIWIN. .....

†2.3 **DENSITY (relative density)** *(Where applicable, indicate the relative density of the substance.)*

Type: Bulk density **[ ]**; Density **[ ]**; Relative Density **[ ] Specific Gravity**

Value: 0.97-1.01 .....
Temperature: . . . . . °C
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: BFGoodrich MSDS .....

***2.4 VAPOUR PRESSURE** *(if more than one, identify the recommended value)*

Value: 9.99E-007 to 1.9E-015. . . . . hPa
Temperature: . . . . . °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updated of the method used)].
EPIWIN. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: .Range for components .....
Reference: .EPIWIN .....

***2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$** *(if more than one, identify the recommended value)*

Log Pow: 5.2
Temperature: Room Temperature, 21 °C
Method: calculated **[ ]**; measured **[** x **]**
[e.g. OECD, other (with the year of publication or updating of the method used)].
OECD Section 1 N0. 107; EEC Annex V Test Guideline A.*., September 19, 1984..
GLP: Yes **[ ]** No **[x]** ? **[ ]**
Remarks: . .....
Reference: BFGoodrich Co., Brecksville R&D Center, November 28, 1990

PARTITION COEFFICIENT $\log_{10}P_{ow}$ *(if more than one, identify the recommended value)*

Log Pow: 5.45 to 15.13
Temperature: Room Temperature, 21 °C
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)].
EPIWIN .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: EPIWIN

***2.6 WATER SOLUBILITY** *(if more than one, identify the recommended value)*

A. Solubility

Value: Negligible. . . . . .
Temperature: . . . . . °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;

Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: BFGoodrich MSDS. .....

Solubility

Value: 0.3889 to 1.869e-011. . . . . .

Temperature: 25. . . . . °C

Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*

EPIWIN. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: .Range for components .....

Reference: EPIWIN. .....

B. pH Value, pKa Value

pH Value: . . . . . .

Concentration: . . . . . .

Temperature: . . . . . °C

Method: *[e.g. OECD, other (with the year of publication or updating of the method used).*

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

(Where applicable, enter values for the dissociation constant(s) and the conditions under which they were measured.)

pKa value . . . . . at 25°C

Remarks: . .....

Reference: . .....

2.7 FLASH POINT *(liquids)*

Value: 180 °C

Type of test: Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**

Method: *(with the year of publication or updating of the method used).* .....

. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Remarks: . .....

Reference: .BFGoodrich MSDS .....

2.8 AUTO FLAMMABILITY *(solid/gases)*

Value: . . . . . °C
Pressure: . . . . . hPa
Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.9 FLAMMABILITY

Results: Extremely flammable **[ ]**; Extremely flammable - liquified gas **[ ]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.10 EXPLOSIVE PROPERTIES

Results: Explosive under influence of a flame**[ ]**;
More sensitive to friction than m-dinitrobenzene **[ ]**;
More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**;
Other **[ ]**
Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;
Vigorous reaction in preliminary test **[ ]**;
No oxidising properties **[ ]**; Other **[ ]**

Method: *(with the year of publication or updating of the method used)*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

†2.12 OXIDATION: REDUCTION POTENTIAL

(Where applicable, indicate the redox potential and the conditions under which it was measured.)

Value: . . . . . mV

Method: *(with the year of publication or updating of the method used)*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value: . . . . . .
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: . .....
Reference: . .....

B. Other data

(e.g. Henry's Law constant, fat solubility, surface tension (of aqueous solution), adsorption/desorption on soil, particle size distribution, etc.)

Results: . .....
Remarks: . .....
Reference: . .....

3. <u>ENVIRONMENTAL FATE AND PATHWAYS</u>

[Reporting of studies should give the test method, test conditions (laboratory versus field studies), test results (e.g. % degradation in specified time period) and reference. Information on breakdown products (transient and stable) should be provided when available.]

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air **[x]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: . . . . . nm
Relative intensity: . . . . . *(based on intensity of sunlight)*
Spectrum of substance: *[e.g. lambda (max.)(>295nm) and epsilon (max) or epsilon (295nm)]*
. . . . . nm
Concentration of Substance: . . . . . .
Temperature: . . . . . °C
Direct photolysis:
Half life: 0.051 to 0.053 days. . . . . .
Degradation: . . . . . % (weight/weight) after . . . . . (exposure time)
Quantum yield: . . . . . .
Indirect Photolysis:
Type of sensitizer: . . . . . .
Concentration of sensitizer: . . . . . .
Rate constant (radical): . . . . . cm^3/molecule*sec

Degradation: . . . . . .
Method: calculated **[ ]**; measured **[ ]**
[e.g. OECD, other (with the year of publication or updating of the method used)]
EPIWIN.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity:. . . . . .
Remarks: .....
Reference: .EPIWIN.....

***3.1.2 STABILITY IN WATER**

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life: . . . . . at pH . . . . . at . . . . . °C
Degradation: . . . . . at pH . . . . . at . . . . . °C after
. . . . . (exposure time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: *(e.g. CAS number, name and percentage of degradation products)*
.....
Reference: .....

3.1.3 STABILITY IN SOIL

Type : Field trial **[ ]**; Laboratory **[ ]**; Other **[ ]**
Radiolabel: Yes **[ ]** No **[ ]** ? **[ ]**
Concentration: . . . . . .
Soil temperature: . . . . . °C
Soil humidity: . . . . . .
Soil classification: DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[ ]**
year . . . . . .
Content of clay etc.: Clay . . . . . %, Silt . . . . . %, Sand . . . . . %
Organic Carbon: . . . . . .
Soil pH: . . . . . .
Cation exchange capacity: . . . . . .
Microbial biomass: . . . . . .
Dissipation time: DT 50 : . . . . . .
DT 90 : . . . . . .
Dissipation : . . . . . % after . . . . . (time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

*3.2 MONITORING DATA (ENVIRONMENTAL)

Note that data on biological effects monitoring, including biomagnification, and biotransformation and kinetics in environmental species are to be reported in section 4.7 and 4.8, respectively. Nonetheless, concentration in various biota should be reported here. Data on concentration in the workplace or indoor environment should be reported under item 5.11.

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**
Media: .....
Results: .....
Remarks: .....
Reference: .....

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

(e.g. during the chemical life-cycle. The information should indicate whether the calculation is on a global basis or is site-specific, and whether it is based on laboratory measurements or field observations.)

*3.3.1 TRANSPORT

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media: .....
Method: .....
Results: .....
Remarks: .....
Reference: .....

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**;
Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**
Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[x]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**
EPIWIN.....
Results: Air 0.0568% to 0.00992%, 1.27 hr to 1.23 hr. half-life, 1000 kg/hr
Water 13.5% to 1.26%, 900hr to 1.44e+003hr half-life, 1000 kg/hr
Soil 44% to 28.6%, 900hr to 1.44e+003, 1000 kg/hr
Sediment 42.5% to 69%, 3.6e+003 to 1.44e-004 half'life, 0 kg/hr.....
Remarks: .....
Reference: .EPIWIN.....

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

Results: .....
Remarks: .....
Reference: .....

*3.5 BIODEGRADATION

Type: aerobic **[ ]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[ ]**; .....
Concentration of the chemical: . . . . . related to COD **[ ]**; DOC **[ ]**; test substance **[ ]**
Medium: water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation: *(percentage reduction/exposure time)*
. . . . . % after . . . . . (time)
Results: *(see OECD Guidelines)* readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic (e.g. Zahn-Wellens-Test) . . . . . % in . . . . . (time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: *[In the case of poorly soluble chemicals, treatment given (nature, concentration, CAS number, name and percentage of degradation products etc.)]:*. .....
. .....
Reference: . .....

3.6 BOD_5, COD OR RATIO BOD_5/COD

BOD_5
Method: . . . . . .
Concentration: . . . . . related to COD **[ ]**; DOC **[ ]**; Test substance **[ ]**
Value: . . . . . mg O_2/l
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

COD
Method: . . . . . .
Value: . . . . . mg O_2/g
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Ratio BOD_5/COD: . . . . . .
Remarks: . .....
Reference: . .....

3.7 BIOACCUMULATION

Species: . .....
Exposure period: . .....
Temperature: . . . . . °C
Concentration: . . . . . .
BCF: . . . . . .
Elimination: Yes **[ ]** No **[ ]** ? **[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....

Type of test: calculated **[ ]**; measured **[ ]**
static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity:. . . . . .

Remarks: . .....

Reference: . .....

3.8 ADDITIONAL REMARKS

A. Sewage treatment *(information on treatability of the substance)*

Results: . .....

Remarks: . .....

Reference: . .....

B. Other information *[information that will help to focus the exposure assessment (either qualitative or quantitative)]*

Results: . .....

Remarks: . .....

Reference: . .....

4. <u>ECOTOXICITY</u>

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
open-system **[ ]**; closed-system **[ ]**

Species: . .....

Exposure period: . .....

Results: LC_{50} (24h) = ... mg/l
LC_{50} (48h) = ... mg/l
LC_{50} (72h) = ... mg/l
LC_{50} (96h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)].*
. .....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: . .....

Reference: . .....

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Exposure period: . .....
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (..h) = ... mg/l
NOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

B. Other aquatic organisms

Type of test: static **[ ]**; semi-static **[x]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: .Mysid shrimp .....
Exposure period: .96 hr. .....
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (.96h) = . . .2.3 . . . . . mg/l
NOEC = ... <1.3. . . . . mg/l
Analytical monitoring: Yes **[x]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
.OECD Guidelines 471 B14 in EC Directive 92/69/EEC
GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance:. . .!00% acitive ingredient . . . . . , purity: . . . . . .
Remarks: . .....
Reference: .Springborn Laboratories, Inc. Report #89-11-3144 (January 10, 1990) ....

*4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae

Species: . .....
Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[ ]**
Exposure period: . .....
Results: . . . . . EC_{50} (. . . . . .h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . .h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
open-system **[ ]**; closed-system **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.4 TOXICITY TO BACTERIA *(Single species tests and tests on overall processes such as nitrification or soil respiration are included in this item.)*

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: . .....
Exposure Period: . .....
Results: EC_{50} (. . . h) = ... mg/l
EC_{xx} (. . . h) = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used*
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH (*effects on reproduction, embryo/larva, etc.*)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: . .....
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[ ]**
Exposure period: . .....
Results: . . . . . EC_{50} (..d) = ... mg/l
(Endpoint) EC_{xx} (..d) = ... mg/l
NOEC = ...mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*. .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

(*)4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES *(e.g. daphnia reproduction. The need to conduct tests for this endpoint will depend inter alia upon possible concern for long term effects.)*

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: .....
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period: . . . . . .
Results: . . . . . EC_{50} (. . . . . h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . d) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[ ]**
Species: .....
Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period: .....
Results: . . . . . EC_{50} (. . . . . d) = ... mg/kg
(Endpoint) EC_{50} (. . . . . d) = ... mg/kg
EC_{xx} (. . . . . d) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)

Species: .....

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**

Exposure period: .....

Results: EC_{50} and/or LC_{50} (7d) = ... mg/l

EC_{50} and/or LC_{50}(14d) = ... mg/l

EC_{xx} and/or LC_{xx} (xxd) = ...mg/l

NOEC = ...mg/l

LOEC = ...mg/l

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....

.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

(b)

Species: .....

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**

Exposure period: .....

Results: EC_{50} and/or LC_{50} (7d) = ... mg/l

EC_{50} and/or LC_{50}(14d) = ... mg/l

EC_{xx} and/or LC_{xx} (xxd) = ...mg/l

NOEC = ...mg/l

LOEC = ...mg/l

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....

.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

(c)

Species: ..... .

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**

Exposure period: .....

Results: EC_{50} and/or LC_{50} (7d) = ... mg/l

EC_{50} and/or LC_{50}(14d) = ... mg/l

EC_{xx} and/or LC_{xx} (xxd) = ...mg/l

NOEC = ...mg/l

LOEC = ...mg/l

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....

.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance:. . . . . , purity: . . . . . .

Remarks: .....

Reference: .....

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species: .....
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period: .....
Results: LD_{xx} or LC_{xx} (xxd) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:....., purity: .....
Remarks: .....
Reference: .....

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

(Studies on variation of predominant species in certain ecosystems (e.g. mesocosm) and monitoring of biological effects are included.)

Results: Substance:.....
Species or ecosystem studied: .....
Effects monitored: .....
Results:.....
Chemical analysis:.....
Remarks: *(Information on environmental conditions (e.g. water characteristics: suspended matter, pH, temperature, hardness; soil/sediment characteristics: % organic matter, clay content)*
.....
Reference: .....

4.8 BIOTRANSFORMATION AND KINETICS

(Under this item, studies on absorption, distribution, metabolism and excretion etc. should be given.)

Type: Animal **[ ]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Results: .....
Remarks: .....
Reference: .....

4.9 ADDITIONAL REMARKS

Results: .....
Remarks: .....
Reference: .....

5. TOXICITY

(Where observations on humans are available, these should be entered in the appropriate "Comments" section or under section 5.11.)

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Value: . . . . . mg/kg b.w.:
Discriminating dose: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Exposure time: .....
Value: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Value: . . . . . mg/kg b.w.
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION
(e.g. subcutaneous, intravenous, etc.)

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: .....
Route of Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time: .....
Value: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain: .....
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: *(If possible, according to EC Directive 67/548/EEC)*
Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[ ]**; Not irritating **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.2.2 EYE IRRITATION/CORROSION

Species/strain: .....
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.3 SKIN SENSITISATION

Type: Human Patch Test.....
Species/strain: Humans
Results: Sensitizing **[ ]**; Not sensitizing **[x]**; Ambiguous **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Sensitizing **[ ]**; Not sensitizing **[ ]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
Shalanski Patch Test
GLP: Yes **[ ]** No **[x]** ? **[ ]**
Test substance: BFGoodrich Material No. 2 (Stalite) , purity: Unknown
Remarks: .....
Reference: Morris V. Shalanski, 1953

*5.4 REPEATED DOSE TOXICITY

Species/strain: Rat/Carworth
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[x]**; No data **[ ]**
Route of Administration: Dietary
Exposure period: 64 weeks
Frequency of treatment: Daily
Post exposure observation period: None
Dose: 2,500, 5,000, and 10,000 ppm
Control group: Yes **[x]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[x]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL: Not Identified
LOEL: 2500 ppm
Results: Daily dietary administration significantly retarded growth in females at 2500 ppm and higher. No effect on growth occurred in males at 2500 ppm. Liver enlargement was noted at all concentrations in both sexes. Diffuse hepatic degeneration was observed in all test animals. However, the severity of the liver changes were not treatment-related. No compound-related hematopoietic changes were observed in any of the test groups.
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*.....
.....
GLP: Yes **[ ]** No **[** x **]** ? **[ ]**
Test substance: Compound 3190 , purity: Unknown
Reference: Treon et al. (1957). The Kettering Laboratory, University of Cincinnati

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: *Bacterial reverse mutation assay*

System of testing: *Salmonella typhymurium*, strains TA-1535, TA-1537, TA-98, TA-100 and *Escherichia coli* strain WP2uvrA-

Concentration: 50, 150, 500, 1500, 5000 ug/plate .....
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[x]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: None toxic
Without metabolic activation: None toxic
Precipitation conc: 1500 and 5000 ug/plate
Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[x]**
Without metabolic activation:	**[ ]**	**[ ]**	**[x]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
OECD 471 B14 in EC Directive 92/69/eec
GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance: Vanlube® SL, purity: .98 %
Remarks: .....
Reference: Safepharm Laboratories Limited, Project No. 860/032, 17 December 1997

B. NON-BACTERIAL IN VITRO TEST

Type: *(e.g. mammalian cell gene mutation assay, cytogenetic assay, etc.)*
. .....
System of testing: . .....
Concentration: . .....
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[ ]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation:. .....
Without metabolic activation:. .....
Precipitation conc: . .....
Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[ ]**
Without metabolic activation:	**[ ]**	**[ ]**	**[ ]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
. .....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

* 5.6 GENETIC TOXICITY IN VIVO

Type: *(e.g. micronucleus assay, etc.)*
.....
Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: .....
Doses: .....
Results:
Effect on mitotic index or P/N ratio: .....
Genotoxic effects: + ? -
[ ] [ ] [ ]
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

5.7 CARCINOGENICITY

Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .....
Exposure period: .....
Frequency of treatment: .....
Postexposure observation period: .....
Doses: .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**; Other **[ ]**
Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:.....
Exposure period: .....
Frequency of treatment: .....
Post exposure observation period: .....
Premating exposure period: male: . . . . . , female: .....
Duration of the test: .....
Doses: .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Parental: .....
NOEL F1 Offspring: .....
NOEL F2 Offspring: .....
Results: .....
General parental toxicity:.....
Toxicity to offspring: *(weights of litter, postnatal growth, viability, etc.)*
.....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: .....
Reference: .....

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species/strain: .....
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: ..... .
Duration of the test: .....
Exposure period: .....
Frequency of treatment: .....
Doses: .....
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Maternal Toxicity: .....
NOEL teratogenicity : .....
Results: .....
Maternal general toxicity:.....
Pregnancy/litter data:.....
Foetal data: .....
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:. . . . . , purity: . . . . . .
Remarks: . .....
Reference: . .....

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: *(e.g. neurotoxicity, immunotoxicity, etc.)*
. .....
Results: . .....
Remarks: . .....
Reference: . .....

B. Toxicodynamics, toxicokinetics

Type: *(e.g. toxicodynamics, toxicokinetics)*
. .....
Results: . .....
Remarks: . .....
References: . .....

I U C L I D

D a t a S e t

Existing Chemical	ID: 122-39-4
CAS No.	122-39-4
EINECS Name	diphenylamine
EINECS No.	204-539-4
TSCA Name	Benzenamine, N-phenyl-
Molecular Formula	C12H11N

Producer Related Part
  Company: EUROPEAN COMMISSION - European Chemicals Bureau
  Creation date: 11-FEB-2000

Substance Related Part
  Company: EUROPEAN COMMISSION - European Chemicals Bureau
  Creation date: 11-FEB-2000

Printing date:	02-NOV-2001
Revision date:	11-FEB-2000
Date of last Update:	09-MAY-1994

Number of Pages: 45

Chapter (profile):	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8, 5.9
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 Melting Point

Value: 52.5 - 55.5 degree C
Source: Bayer AG Leverkusen
(18)

2.2 Boiling Point

Value: ca. 159 degree C at 122 hPa
Source: Bayer AG Leverkusen
(83)

Value: ca. 261 degree C at 400 hPa
Source: Bayer AG Leverkusen
(83)

Value: 302 degree C at 1013 hPa
Source: Bayer AG Leverkusen
(18)

2.4 Vapour Pressure

Value: .000215 hPa at 20 degree C
Source: Bayer AG Leverkusen
(18)

Value: 1.3 hPa at 108 degree C
Source: Bayer AG Leverkusen
(18)

2.5 Partition Coefficient

log Pow: 3.5
Method:
Year:
Remark: measured
Source: Bayer AG Leverkusen
(96)

log Pow: 3.6
Method: other (calculated): Leo, Hansch: A. Leo, CLOGP-3.63 (1991)
Daylight, Chemical Information Systems, Inc. Irvine, CA, USA
Year:

Source: Bayer AG Leverkusen

(19)

2.6.1 Water Solubility

Value: .04 g/l at 25 degree C
Source: Bayer AG Leverkusen

(18)

Value: ca. .05 g/l at 25 degree C
Source: Bayer AG Leverkusen

(83)

3.1.1 Photodegradation

Type: water
Method:
Year: GLP:
Test substance:
Remark: Rapid photodegradation in water is to be expected.
Source: Bayer AG Leverkusen

(18)

3.1.2 Stability in Water
-

3.3.1 Transport between Environmental Compartments
-

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Degradation: 0 % after 14 day
Result: other: no degradation
Method:
Year: GLP: no data
Test substance:
Remark: "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).
Sludge conc. : 30 mg/l
Source: Bayer AG Leverkusen

(16)

Type:
Inoculum:
Result: other: no degradation
Method: other: diverse
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen

(18)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 20
Method: other: Bestimmung der akuten Wirkung von Stoffen auf Fische. Arbeitskreis "Fischtest" im Hauptausschuss "Detergentien" (15.10.73)
Year: 1973 GLP: no
Test substance:
Remark: range finding test
Source: Bayer AG Leverkusen

(14)

Type:
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 2.2
Method: other: JIS K0102, Japanese Industrial Standards Commitee (1971)
Year: GLP: no data
Test substance:

Remark: dissolved in 1 ml of ethanol and then diluted with water
Source: Bayer AG Leverkusen

(97)

Type:

Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 5.1
Method: other: Japanese Industrial Standard (JIS K 0102-1986-71) "Testing methods for industrial waste water"
Year: GLP: no data
Test substance:
Source: Bayer AG Leverkusen

(16)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 2.3
Method: other: Immobilization test, UBA-Verfahrensvorschlag Mai 1984, Bestimmung der Schwimmunfaehigkeit beim Wasserfloh Daphnia magna, EC0, EC50, EC100 24h, statisches System
Year: 1986 GLP: no
Test substance:
Source: Bayer AG Leverkusen

(18)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: other: cell count
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: .048
Method: other: UBA-Verfahrensvorschlag "Hemmung der Zellvermehrung bei der Gruenalge Scenedesmus subspicatus" (EC 10, EC 50; 72 h; statisches System)
Year: 1986 GLP: no
Test substance:
Source: Bayer AG Leverkusen

(18)

Species: Scenedesmus subspicatus (Algae)
Endpoint:
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: yes
Method: other: Test guideline "Algeninhibitionstest" (C.3) Directive 67/548/EEC (Draft 1992)
Year: 1992 GLP: yes
Test substance: other TS: 99.7 %
Remark: biomass
EC 10 : 0.01 mg/l

EC 50 : 0.18 mg/l
growth rate
EC 10 : 0.06 mg/l
EC 50 : 1.50 mg/l
Dunnett-Test (Basis: cell count after 72 h)
NOEC : 0.02 mg/l
LOEC : 0.04 mg/l
Nominal concentration
Analytical monitoring: HPLC

Source: Bayer AG Leverkusen

(14)

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 1165 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen

(68)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 3200 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen

(36)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:

Vehicle:
Value: = 3200 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(105)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(69) (70)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 2000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(62)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 2960 mg/kg bw
Method:
Year: GLP:
Test substance:
Remark: sex: male
Source: Bayer AG Leverkusen
(90)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 2480 mg/kg bw
Method:
Year: GLP:
Test substance:
Remark: sex: female
Source: Bayer AG Leverkusen

(90)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: >= 1500 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Uniroyal Chemical Company, Middelebury, USA
Bayer AG Leverkusen

(98)

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 1750 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen

(62)

Type: LD50
Species: guinea pig
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 300 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(73)

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(68)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 2000 mg/kg bw
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(101)

5.1.4 Acute Toxicity, other Routes
-

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: no data
Route of admin.: oral feed
Exposure period: 734 d
Frequency of treatment: daily
Post. obs. period: no data
Doses: 0.001, 0.01, 0.1, 0.5 or 1 % = ca. 0.7, 6.7, 67, 333 or 667 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance: other TS: "virtually 100 % pure with a minimum purity of 99.9 %"
Result: all dose levels: good survival at 640 and 734 d, no significant reduction in the number of survivors
dose levels up to and including 0.1 %: no growth inhibition during the first 240 d
0.1-0.5 %: histopathological changes in animals killed from 640 d: cystic dilated renal tubules accompanied by chronic interstitial nephritis
0.5 and 1 %: distinct growth inhibition
1 %: decrease in food consumption by more than 10 %; haematology (observation period: 126-463 d): moderate degree of anaemia (reduction in haemoglobin and red cell levels, increased number of circulating normoblasts)
Source: Bayer AG Leverkusen

(31)

Species: rat Sex: male
Strain: no data
Route of admin.: oral feed
Exposure period: 19 w
Frequency of treatment: daily
Post. obs. period: no data
Doses: 2.5 % (= ca. 1667 mg/kg bw/d)
Control Group: other: no data
Method:
Year: GLP:
Test substance:
Remark: similar changes could also be obtained in mice dosed with diphenylamine (no further data)
Result: the earliest histological changes of the kidneys were seen in the epithelial cells of the proximal tubule and consisted of a marked increase in the number and size of electron dense bodies; subsequently a few proximal tubule cells degenerated; in the collecting and distal tubules the first changes also appeared to be an increase in number and size

of electron dense bodies; other manifestations of cellular degeneration were vacuolisation and swollen mitochondria;

the epithelial cells of the distal tubules sloughed off leaving naked basement membrane; fibroblasts were seen arranging themselves circumferentially externally to the basement membrane; the place of the original tubular epithelium was taken by the fibroblast, which in turn degenerated and sloughed off into the tubular lumen being replaced by successive generations; at times the walls of the renal cysts were seen to be several layers thick, the innermost layers showing the most degeneration;
results of microdissection studies: the earliest changes occurred at about 6 w and consisted of a flattening of the epithelium of the distal convoluted and connecting tubule; at 10 w some of the nephrons showed that the lumen was increased in diameter and the whole tubule became dilated; at 15 w the changes appeared both in the distal and collecting tubule and spread to the upper nephron, in many areas the tubules had become cystic and many more of the nephrons were now affected; at 19 w there was merely extension and accentuation of the whole process

Source: Bayer AG Leverkusen

(29) (30) (110)

Species: rat Sex: male
Strain: no data
Route of admin.: oral feed
Exposure period: 30 d
Frequency of treatment: daily
Post. obs. period: no data
Doses: 100, 1000 or 10000 ppm (= ca. 6.7, 67 or 667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: no histological examination was made of the tissues
Result: all dose levels: no deaths
100 and 1000 ppm: no signs of toxicity; results of the autopsy: no gross pathologic lesions that could be attributed to feeding of diphenylamine
1000 ppm: food intake and weight gain significantly higher compared with those of the controls
10000 ppm: only about one-half the weight gain of the controls (the food intakes not differing from the controls); results of the autopsy: dark and roughened spleens, hyperaemic kidneys in 3/10 animals; paleness of the extremities in most of the rats (no chemical analysis was performed to determine if methaemoglobin was present in the

blood)
Source: Bayer AG Leverkusen

(7)

Species: rat Sex: no data
Strain: Wistar
Route of admin.: oral feed
Exposure period: 217 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 10 mg sodium nitrite/rat/d and 5 mg diphenylamine/rat/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: 3/25 animals were sacrificed every 30 d; the organs were examined histologically and the stomach and liver were analysed for nitrosamines
the diet contained 0.04 % sodium nitrite and 0.02 % diphenylamine
Result: impaired growth of the animals, nitrosodiphenylamine chromatographically identifiable in the stomach of the rats; histological damage: vacuolisation and clear swelling of the hepatic cells, variation in the size of the nuclei, focal necrosis surrounded by inflammatory cells; papillomatous hyperplasia apparent in the bladder, associated with a chronic interstitial nephritis
Source: Bayer AG Leverkusen

(44)

Species: rat Sex: female
Strain: no data
Route of admin.: oral feed
Exposure period: 226 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 0.025, 0.1, 0.5, 1.0 or 1.5 %
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: doses: 0.025, 0.1, 0.5, 1.0 or 1.5 % = ca. 17, 67, 333, 667 or 1000 mg/kg bw/d
Result: 0.5 % or more: inhibition of growth, focal dilatation of renal tubules and cyst formation in the kidneys
Source: Bayer AG Leverkusen

(93)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: up to 12 months
Frequency of treatment: daily
Post. obs. period: no data
Doses: 2.5 % (= ca. 1667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: studies were performed on rats of 2 age groups: weanling rats of both sexes and adult male rats
Result: acquired form of polycystic renal disease: development of cystic changes appearing to be the result of proximal tubular epithelial cell degeneration coupled with luminal narrowing of distal tubules; decrease in glomerular filtration rate and in maximal urinary osmolality; polycystic kidneys having a markedly increased susceptibility to pyelonephritis
Source: Bayer AG Leverkusen
(61)

Species: rat Sex: male/female
Strain: other: Slonaker-Addis
Route of admin.: oral feed
Exposure period: 2 years
Frequency of treatment: daily
Post. obs. period: no
Doses: 0.001, 0.01, 0.10, 0.50 or 1.0 % = ca. 0.7, 6.7, 67, 333 or 667 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Result: 0.1 % or more: inhibition of growth of the females
ca. 0.1 % = "break-point" for the occurrence of a cystic dilatation of the renal tubules
0.1-0.5 %: break-point for the occurrence of chronic

nephritis clearly lying within this dose range
0.5 and 1.0 %: inhibition of growth of the males; moderate degrees of anaemia
Source: Bayer AG Leverkusen
(94)

Species: rat Sex: no data
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: up to 12 months
Frequency of treatment: daily
Post. obs. period: no data
Doses: 1.5 or 2.5 % (= ca. 1000 or 1667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was added to the diets of various groups of rats as follows: group 1 received 1.5 %; group 2 received 2.5 %; group 3 received 1.5 % diphenylamine supplemented with 0.25 % sulfur-containing amino acids (equal amounts of d,l-methionine and l-cystine); group 4 received 2.5 % diphenylamine supplemented with 0.5 % of the same sulfur-containing amino acids
no explanation for the additive effect of sulfur-containing amino acids is available, but in the authors opinion it is possible that the acidosis induced by the amino acids might enhance the injury induced by diphenylamine to the renal tubule
Result: both dose levels: cystic renal changes
2.5 %: the mean maximal urinary concentrating ability was reduced before gross pathologic defects were discernible; sulfur-containing amino acids significantly increased the degree of cystic changes producing the most severe examples of diffuse cystic renal disease encountered in the entire group of animals
Source: Bayer AG Leverkusen

(84)

Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 12 to 18 months
Frequency of treatment: daily
Post. obs. period: no data
Doses: 1 % (= ca. 667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:

Test substance:

Remark: number of test animals: 3
Result: renal cystic disease: changes in the renal corpuscles, including dilation of Bowmans space, podocyte fusion and degeneration and basement membrane thickening; cysts being present along the entire nephron; collecting duct cysts lined by cells of irregular size and shape suggestive of cell hypertrophy and/or hyperplasia; cast material identi-

fiable in the cysts; atrophy of a few renal corpuscles
Source: Bayer AG Leverkusen

(38)

Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 5-20 months
Frequency of treatment: daily
Post. obs. period: no data
Doses: 1 % (= ca. 667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: it was concluded by the author that the elevated hydrostatic pressures in the dilated nephrons were the consequence of variably severe and frequently incomplete tubular occlusion; the findings support the hypothesis that renal cyst formation is a consequence of partial obstruction and elevated intratubular pressure
Result: heterogeneous renal lesions: dilation and frank cyst formation occurring in 5-30 % of nephrons; elevated intraluminal hydrostatic pressures detectable in dilated, but not in nondilated nephrons; structural studies demonstrate communication of dilated nephrons with cysts, concretions of debris within tubular lumens, apparent luminal narrowing of some proximal tubules, evidence of extrinsic pressure by cysts on adjacent tubules; these observations were used to explain prolonged loop of Henle transit times and occasional failure to detect 3H-inulin excretion after microperfusion into dilated tubules
Source: Bayer AG Leverkusen

(45)

Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: up to 18 months
Frequency of treatment: daily
Post. obs. period: no data
Doses: 1 % (= ca. 667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: the author states that the hyperplasia of the renal collecting tubules on the one hand and the sites of partial obstruction along the collection tubule on the other hand cause the tubules to dilate
Result: urinary concentrating defect associated with reduced renal papillary urea concentration and increased urine flow (urinary osmolality significantly decreased at 6 and 20 w); hyperplastic change at 5 w in cells of the renal medullary collecting ducts: multilayering of cells, increase in the number of nuclei, relative increase in the number of 3H-thymidine-labeled nuclei; by 10 w, dilation of some collecting ducts with focal areas of cellular necrosis, a small amount of cast material detectable in a few collecting ducts; by 15 to 20 w, numerous collecting ducts being dilated and containing cast material and by 24 w, frank cysts observable in the renal cortex and medulla; by 1 to 2 years, frank cysts discernible in every segment of the nephron and collecting tubules; by 1 year, many large cysts in the collecting tubules (cysts usually filled with necrotic cast material); by 1 to 2 years, numerous areas of chronic inflammation discernible, with a concomitant loss of nephrons
Source: Bayer AG Leverkusen

(39) (40)

Species: rat Sex: male/female
Strain: Wistar
Route of admin.: oral feed
Exposure period: 6 months
Frequency of treatment: daily
Post. obs. period: no
Doses: 2 or 4 % (= ca. 1333 or 2667 mg/kg bw/d)
Control Group: yes
Method:

Year: GLP:
Test substance: other TS: technical diphenylamine containing 0.5 % aromatic amines (aniline and amino-4-diphenyl) as impurities
Remark: 4 experimental animals per test group were used: 1 male, 2 pregnant females and 1 non-pregnant female
four experimental groups were used: group 1 received 2 % of diphenylamine in the diet; group 2 received 4 % of diphenylamine; group 3 received 2 % of diphenylamine and additionally 0.5 % of amino acids (D-L-methionine and L-cystine in equal shares); group 4 received 4 % of diphenylamine and 0.5 % of the amino acids mentioned above
in the same study guinea pigs were also used; they showed greater sensitivity to intoxication with diphenylamine than the rats
Result: all dose levels: cystic dilatation of the renal tubules (dose-dependent); general condition of the animals rapidly impaired (especially in the 4 %-group); after 1-2 w occurrence of pulmonary oedema; hair loss, decreased spontaneous activity, early end of gestation; death of 17 animals in the course of the first month of the study; hepatocellular necrosis (the amino acids which were added to some of the diets did not reveal any protective effect)
Source: Bayer AG Leverkusen

(75)

Species: rat Sex: female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 3 to 6 w
Frequency of treatment: daily
Post. obs. period: no data
Doses: 2.5 % (= ca. 1667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Result: significant defect in maximal urine concentrating ability (manifest by the second week and averaging 50 % of control values); morphological examination of the kidneys: gross cysts identifiable in the corticomedullary region in approximately 10 % of all kidneys examined; histological examination of the kidneys: morphological alterations in all the kidneys of the experimental animals, cystic dilatation of the collecting ducts (the most consistent finding, most marked in the medullary region of the kidney), proteinaceous casts occasionally observable within the dilated tubules, focal dilatation of the cortical collecting ducts and distal tubules (less consistently

seen); glomeruli, proximal tubules and interstitium appearing morphologically normal
Source: Bayer AG Leverkusen

(34)

Species: rat Sex: no data
Strain: no data
Route of admin.: oral feed
Exposure period: up to 15 months
Frequency of treatment: daily
Post. obs. period: no data
Doses: 2.5 % (= ca. 1667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: the animals were sacrificed after an experimental period of 6, 12 or 15 months
Result: results of light microscopy studies of the kidneys: a marked disorganization of the renal pyramid structure was evident in all kidneys; both the juxtacortical portion as well as the papilla proper were affected; vacuolation of the tubular walls leading to cyst formation, was a common finding
Source: Bayer AG Leverkusen

(3)

Species: rat Sex: male
Strain: other: Carworth Europe CFY, C.D.; Charles River C.D.; Sprague Dawley CFY
Route of admin.: gavage
Exposure period: 14 d
Frequency of treatment: daily
Post. obs. period: no data
Doses: doses exceeding approximately 2 mmol/kg bw (338 mg/kg bw)
Control Group: yes
Method:
Year: GLP:
Test substance:
Result: well delineated necrosis of some 20 % of the renal papillary apex, reduced capacity to concentrate urine, polyuria, pronounced azotaemia, reduced ability to secrete an acid urine following oral ammonium ion load, grossly elevated absolute kidney weights
Source: Bayer AG Leverkusen

(54)

Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 3 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in peanut oil prior to application
Result: 600 mg/kg bw/d: gross lesion: bilateral renal cortical pallor in 1/10 rats
800 mg/kg bw/d: renal papillary lesions: apex-limited necrosis of the medullary interstitial cells and vasa recta and degeneration of the renal interstitial matrix in 2/10 rats
Source: Bayer AG Leverkusen

(67)

Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 9 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in dimethylsulphoxide prior to application
Result: all dose levels: gross renal lesions (brown kidney); no significant microscopic lesions observable in sections of liver, pancreas, myocardium or lung
800 mg/kg bw/d: focal, apex-limited (early) renal papillary necrosis in 2/30 rats; focal, intermediate renal papillary necrosis observable in additional 2/30 rats; microscopic lesions of the outer medulla or renal cortex not observable
Source: Bayer AG Leverkusen

(66)

Species: rat Sex: male
Strain: no data
Route of admin.: oral unspecified
Exposure period: no data
Frequency of treatment: daily
Post. obs. period: no data
Doses: 0.05, 0.5 or 5 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: a chronic experiment was performed (no further data concerning the exposure period)
Result: 0.05 and 0.5 mg/kg bw/d: no toxic effects
5 mg/kg bw/d: diphenylamine disturbed the conditioned reflexes, the excretory liver function, the activities of peroxidase and ceruloplasmin and the blood level of SH groups
Source: Bayer AG Leverkusen

(62)

Species: rat Sex: no data
Strain: no data
Route of admin.: oral unspecified
Exposure period: 25 d
Frequency of treatment: daily
Post. obs. period: no data
Doses: 0.2, 0.04 or 0.008 x LD50 (= ca. 400, 80 or 16 mg/kg bw/d)
Control Group: other: no data
Method:
Year: GLP:
Test substance:
Result: no deaths occurred; the test substance exhibited moderate cumulative properties (no further data)
Source: Bayer AG Leverkusen

(62)

Species: rat Sex: male
Strain: Sprague-Dawley
Route of admin.: i.p.
Exposure period: 3 d
Frequency of treatment: daily

Post. obs.
period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in dimethylsulphoxide prior to application
Result: all dose levels: high mortality, no gross renal lesions, no renal papillary necrosis, no significant microscopic lesions in sec- tions of liver, pancreas, myocardium or lung
Source: Bayer AG Leverkusen
(66)

Species: rat Sex: male
Strain: Wistar
Route of admin.: unspecified
Exposure period: 3 d
Frequency of
treatment: daily
Post. obs.
period: 7 d
Doses: 4.1 mmol/kg bw/d (= ca. 694 mg/kg bw/d)
Control Group: other: no data
Method:
Year: GLP:
Test substance:
Result: renal papillary necrosis, proximal straight tubular necrosis and evidence of haemolysis (following a recovery period of 7 d, there was no papillary regeneration, but partial recovery from both the proximal tubular necrosis and the haemolysis were apparent)
Source: Bayer AG Leverkusen
(77)

Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: oral unspecified
Exposure period: 28 d
Frequency of
treatment: daily
Post. obs.
period: 14 d
Doses: 111, 333 or 1000 mg/kg bw/d
Control Group: yes
NOAEL: 111 mg/kg
Method:
Year: GLP:

Test substance:
Result: 111 mg/kg bw/d: no toxic effects
333 mg/kg bw/d: slight increase of spleen, liver and kidney weights as well as slight degeneration of renal tubules observable in several animals
1000 mg/kg bw/d: inhibition of body weight gain; increase of liver, spleen and kidney weights; anaemia; histopathological findings: mucosal hyperplasia in the forestomach; dilatation, degeneration or necrosis of renal tubules in the corticomedullary junction; hyperplasia in the bone marrow (repair of histopathological lesions and anaemia occurred within 14-d resting period)
Source: Bayer AG Leverkusen

(111)

Species: mouse Sex: male/female
Strain: no data
Route of admin.: oral feed
Exposure period: 80 w
Frequency of treatment: daily
Post. obs. period: no data
Doses: 100, 300, 1000 or 5000 ppm (= ca. 14, 43, 143 or 714 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Result: 300 ppm or more: increased mortality
1000 ppm: abnormalities in the spleen
5000 ppm: abnormalities in the liver (chronic inflammatory change, iron pigment deposition), kidneys (iron deposition) and spleen (iron deposition, fibrosis, lymph follicle hypoplasia)
Source: Bayer AG Leverkusen

(99)

Species: mouse Sex: male
Strain: NMRI
Route of admin.: gavage
Exposure period: 10 w
Frequency of treatment: one administration per week
Post. obs. period: ca. 2 months
Doses: 1400 mg/kg bw/w
Control Group: other: no data
Method:
Year: GLP:

Test substance:
Result: death of 5/20 animals within 2 d from the first administration; death of a further 5 animals 2-4 months after the start of the experiment; a total of 10 animals surviving 4.5 months without symptoms of diphenylamine-induced injury; autopsy of the mice who died 3 to 4 months after start of the exposure: severe bilateral change in both kidneys, pale and irregular appearance of the kidneys; microscopical changes in the kidneys and in the liver: renal changes seen all over the kidney but more pronounced in the renal cortex, renal cortices irregularly narrowed and scarred with loss of the normal architecture; the majority of the proximal, distal and collecting tubules either dilated (cystic) or atrophic, many of these tubules containing more or less PAS positive homogeneous or granular material and some of them having also desquamated epithelial cells in their lumen; many glomeruli reduced in size with more or less hyalinized glomerular tufts; increased interstitial connective tissue; activated hepatic reticuloendothelial cells containing a considerable amount of yellowish-brown,

iron-negative pigment in their cytoplasm
Source: Bayer AG Leverkusen
(63) (64)

Species: mouse Sex: male/female
Strain: no data
Route of admin.: s.c.
Exposure period: 80 w
Frequency of treatment: see remarks
Post. obs. period: no data
Doses: see remarks
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: dosage: 0.5 ml of a 25 % solution of diphenylamine in trioctanoin (approximately 4000 mg/kg bw) per application the animals received s.c. injections once every two weeks on alternate sides of the body; after two months it was found that the compound accumulated when given this frequently and the injections were then given once every three weeks until the animals had received injections for a total period of 80 weeks
Result: in this experiment except for one isolated period between weeks 30 and 40 with respect to the female test group, the incidence of mortality was not different from the control group
Source: Bayer AG Leverkusen

(99)

Species: Syrian hamster Sex: male
Strain: no data
Route of admin.: gavage
Exposure period: 3 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in peanut oil prior to application
Result: all dose levels: total renal papillary necrosis (incidences: 4/10 at 400 mg/kg bw/d, 7/10 at 600 mg/kg bw/d, 6/10 at 800 mg/kg bw/d); necrosis of the pars recta not observable 400 mg/kg bw/d: gross lesion: splenomegaly 600 mg/kg bw/d: focal intermediate renal papillary necrosis in 2/10 hamsters; gross lesion: gastric ulcers in 1/10 animals 600 and 800 mg/kg bw/d: gross renal lesions: kidneys swollen and showing a diffuse, dull, brown discoloration

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Source: Bayer AG Leverkusen

(67)

Species: Syrian hamster Sex: male
Strain: no data
Route of admin.: gavage
Exposure period: 9 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in dimethylsulphoxide prior to application
Result: all dose levels: gross renal lesions (brown kidney); no significant microscopic lesions observable in sections of liver, pancreas, myocardium or lung
400 mg/kg bw/d: total renal papillary necrosis in 1/30 animals
Source: Bayer AG Leverkusen

(66)

Species: Syrian hamster Sex: male
Strain: no data
Route of admin.: gavage
Exposure period: 3 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: no
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in peanut oil for this experiment
Result: all dose levels: renal papillary necrosis (incidences: 5/10 at 400 mg/kg bw/d, 7/10 at 600 mg/kg bw/d, 5/10 at 800 mg/kg bw/d)
Source: Bayer AG Leverkusen

(66)

Species: Syrian hamster Sex: male
Strain: no data
Route of admin.: gavage
Exposure period: 3 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: no
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in peanut oil for this experiment; the hamsters were orally administered 0.5 ml dimethylsulphoxide/100 g bw, 1 h before the oral administration of 400, 600 or 800 mg diphenylamine/kg bw/d
Result: all dose levels: no deaths, significantly reduced incidences of renal papillary necrosis (incidences: 0/10 at 400 mg/kg bw/d, 0/10 at 600 mg/kg bw/d, 1/10 at 800 mg/kg bw/d) when compared with hamsters given similar doses of diphenylamine but not pretreated with dimethylsulphoxide
Source: Bayer AG Leverkusen

(66)

Species: Syrian hamster Sex: male
Strain: no data
Route of admin.: i.p.
Exposure period: 3 d

Frequency of
treatment: daily
Post. obs.
period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in peanut oil prior to application
Result: all dose levels: necrosis and degeneration of the renal pars recta (incidences: 7/10 at 400 mg/kg bw/d, 3/10 at 600 mg/ kg bw/d and 4/10 at 800 mg/kg bw/d)
600 and 800 mg/kg bw/d: total renal papillary necrosis (incidences: 5/10 at 600 mg/kg bw/d and 4/10 at 800 mg/kg bw/d); gross renal lesions: kidneys swollen and showing a diffuse, dull, brown discoloration; diffuse renal cortical pallor with congestion of the outer medulla in one hamster from each of the dose levels
800 mg/kg bw/d: focal intermediate renal papillary necrosis in 2/10 hamsters; gross lesions: gastric ulcers in 3/10 hamsters, splenomegaly
Source: Bayer AG Leverkusen

(67)

Species: Syrian hamster Sex: male
Strain: no data
Route of admin.: i.p.
Exposure period: 3 d
Frequency of
treatment: daily
Post. obs.
period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in dimethylsulphoxide prior to application
Result: all dose levels: gross renal lesions (pale renal cortices, brown papilla) and gastric ulcers; total renal papillary necrosis; no significant microscopic lesions observable in sections of liver, pancreas, myocardium or lung
Source: Bayer AG Leverkusen

(66)

Species: dog Sex: male/female
Strain: Beagle

Route of admin.: oral feed
Exposure period: 24 months
Frequency of treatment: daily
Post. obs. period: no data
Doses: 0.01, 0.1 or 1 % (= ca. 8, 77 or 769 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance: other TS: "virtually 100 % pure with a minimum purity of 99.9 %"
Remark: groups made up of 2 dogs of each sex
Result: 0.01 and 0.1 %: up to 400 d no growth inhibition
1 %: severe growth inhibition; haematology: falls in haemoglobin level and red cell count occuring at 724-731 d, blood smears showing crenated red cells, increased fragility of the red cells; liver function tests: increased retention of sulphobromophthalein; increased weight of liver, spleen and kidneys; moderate amounts of intracellular bilirubin in the hepatocytes and some haemosiderosis of the spleen, kidney and bone marrow
Source: Bayer AG Leverkusen

(31)

Species: dog Sex: male/female
Strain: Beagle
Route of admin.: oral feed
Exposure period: 737 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 0.01, 0.10 or 1.0 % (= ca. 8, 77 or 769 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: groups made up of 2 dogs of each sex
minimum purity of the test substance: 99.9 %
Result: 0.1 %: anaemia of mild degree
0.1 and 1.0 %: arrested growth of both sexes
1 %: pronounced anaemia; moderately decreased resistance of the erythrocytes to hypotonicity (after 2 years); sulfobromophthalein tests of liver function from day 618 to day 627 indicate a moderate degree of liver damage; pathology: peripherolobular fatty change in the liver with a marked increase in liver weight and ether-extractable lipids; mild haemosiderosis of the spleen, kidneys and bone marrow; slight increase in kidney weight

Source: Bayer AG Leverkusen

(95)

Species: guinea pig Sex: male/female
Strain: Hartley
Route of admin.: oral feed
Exposure period: 6 months
Frequency of treatment: daily
Post. obs. period: no
Doses: 2 or 4 % (= ca. 800 or 1600 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance: other TS: technical diphenylamine containing 0.5 % aromatic amines (aniline and amino-4-diphenyl) as impurities
Remark: 4 experimental animals per test group were used: 1 male, 2 pregnant females and 1 non-pregnant female
four experimental groups were used: group 1 received 2 % of diphenylamine in the diet; group 2 received 4 % of diphenylamine; group 3 received 2 % of diphenylamine and additionally 0.5 % of amino acids (D-L-methionine and L-cystine in equal shares); group 4 received 4 % of diphenylamine and 0.5 % of the amino acids mentioned above
in the same study rats were also used; they showed less sensitivity to intoxication with diphenylamine than the guinea pigs
Result: all dose levels: cystic dilatation of the renal tubules (dose-dependent); general condition of the animals rapid-

ly impaired (especially in the 4 %-group); after 1-2 w occurrence of pulmonary oedema; hair loss, decreased spontaneous activity, early end of gestation; death of 17 animals in the course of the first month of the study; hepatocellular necrosis (the amino acids which were added to some of the diets did not reveal any protective effect)
Source: Bayer AG Leverkusen

(75)

Species: other: Mongolian gerbil Sex: male
Strain: no data
Route of admin.: gavage
Exposure period: 3 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes

Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in peanut oil prior to application
Result: all dose levels: no gross or microscopic renal lesions observable
Source: Bayer AG Leverkusen
(67)

Species: other: Mongolian gerbil Sex: female
Strain: no data
Route of admin.: gavage
Exposure period: 9 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in dimethylsulphoxide prior to application
Result: all dose levels: no gross renal lesions, no renal papillary necrosis, no significant microscopic lesions in sections of liver, pancreas, myocardium or lung
Source: Bayer AG Leverkusen
(66)

Species: other: Mongolian gerbil Sex: female
Strain: no data
Route of admin.: i.p.
Exposure period: 3 d
Frequency of treatment: daily
Post. obs. period: no
Doses: 50, 100, 200, 400, 600 or 800 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: diphenylamine was dissolved in dimethylsulphoxide prior to application
Result: all dose levels: high mortality, no gross renal lesions, no renal papillary necrosis, no significant microscopic lesions in sections of liver, pancreas, myocardium or lung
Source: Bayer AG Leverkusen
(66)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: S. typhimurium TA 98
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(59)

Type: Ames test
System of testing: S. typhimurium TA 98, TA 100
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method:
Year: GLP:
Test substance:
Remark: experiments were carried out to test the mutagenicity of diphenylamine with and without norharman; diphenylamine was mutagenic to TA 98 in the presence of norharman and S9 mix; the test substance was not mutagenic to TA 98 or TA 100 with or without S9 mix in the absence of norharman

Source: Bayer AG Leverkusen
(92) (107)

Type: Ames test
System of testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen

(71)

Type: Ames test
System of testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:

Test substance:
Remark: the test substance precipitated on the plates; therefore the result obtained with diphenylamine is difficult to evaluate
Source: Bayer AG Leverkusen

(43)

Type: Ames test
System of testing: S. typhimurium TA 100
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen

(12) (35)

Type: Ames test
System of testing: S. typhimurium TA 1538
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen

(41)

Type: Ames test

System of
testing: S. typhimurium G46, TA 1535, TA 1000, C3076, TA 1537, D3052, TA 1538, TA 98
Concentration:
Cytotoxic Conc.:
Metabolic
activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(78)

Type: Ames test
System of
testing: S. typhimurium TA 97, TA 98, TA 100, TA 1535
Concentration:
Cytotoxic Conc.:
Metabolic
activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(113)

Type: Ames test
System of
testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration:
Cytotoxic Conc.:
Metabolic
activation: with and without
Result: positive
Method:
Year: GLP:
Test substance:
Remark: in this assay, the test substance revealed only very weak mutagenicity
Source: Bayer AG Leverkusen
(104)

Type: DNA damage and repair assay
System of
testing: E. coli W3110/polA+ and p3478/polA-
Concentration:
Cytotoxic Conc.:
Metabolic

activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(71)

Type: Escherichia coli reverse mutation assay
System of testing: E. coli WP2 and WP2 uvrA-
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(78)

Type: Mitotic recombination in Saccharomyces cerevisiae
System of testing: Saccharomyces cerevisiae D5
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(71)

Type: Mouse lymphoma assay
System of testing: L5178Y mouse-lymphoma cells
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(4) (5) (6)

Type: Unscheduled DNA synthesis
System of testing: primary cultures of adult rat hepatocytes
Concentration:
Cytotoxic Conc.:
Metabolic activation:
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
(78)

Type: other: DNA-damaging activity
System of testing: Chinese hamster V79 cells
Concentration:
Cytotoxic Conc.:
Metabolic activation: no data
Result: negative
Method:
Year: GLP:
Test substance:
Remark: the generation of DNA single-strand breaks was determined in V79 cells by the alkaline elution assay

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Source: Bayer AG Leverkusen
(47) (48)

Type: other: DNA-damaging activity
System of testing: rat hepatocytes
Concentration:
Cytotoxic Conc.:
Metabolic activation:
Result: positive
Method:
Year: GLP:
Test substance:
Remark: the generation of DNA single-strand breaks was determined in isolated rat hepatocytes by the alkaline elution assay
Source: Bayer AG Leverkusen
(47) (48)

Type: other: SOS chromotest
System of testing: E. coli PQ37

Concentration:
Cytotoxic Conc.:
Metabolic
activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Remark: diphenylamine did not induce SOS-repair in the chromotest with and without S9 mix (without norharman); the addition of norharman to the S9 mix did not influence the negative results
Source: Bayer AG Leverkusen

(106)

5.6 Genetic Toxicity 'in Vivo'

Type: Cytogenetic assay
Species: rat Sex: male
Strain:
Route of admin.: oral unspecified
Exposure period: no data
Doses: 0.05, 0.5 or 5 mg/kg bw/d
Result:
Method:
Year: GLP:
Test substance:
Remark: in a chronic experiment (duration of the administration not specified) the animals received daily oral doses of diphenylamine and at the end of the experimental period bone marrow cell preparations were made and investigated for chromosomal aberrations
type: chromosomal aberration assay
Result: all dose levels: no significant increase in the number of chromosomal aberrations
Source: Bayer AG Leverkusen

(62)

Type: Sister chromatid exchange assay
Species: mouse Sex: male
Strain:
Route of admin.: i.p.
Exposure period: single application
Doses: 1-500 mg/kg bw
Result:
Method:
Year: GLP:
Test substance:
Remark: mouse bone marrow cells were investigated
Result: negative

Source: Bayer AG Leverkusen

(104)

Type: Sister chromatid exchange assay
Species: mouse Sex: no data
Strain:
Route of admin.: i.p.
Exposure period: single application
Doses: 1-100 mg/kg bw
Result:
Method:
Year: GLP:
Test substance:
Result: negative
Source: Bayer AG Leverkusen

(49)

Type: other: Host-mediated assay
Species: mouse Sex: male
Strain:
Route of admin.: gavage
Exposure period: single application
Doses: doses ranging from 1450 to 2900 umoles/kg bw
Result:
Method:
Year: GLP:
Test substance:
Remark: the host-mediated assay was performed with S. typhimurium TA 1950 as genetic indicator system; the bacterial culture was injected i.p. into each mouse and diphenylamine was administered by gavage; injection of the bacteria and p.o. incubation of the test compound were performed simultaneously
Result: results: diphenylamine was without mutagenic activity in the assay when administered alone or together with equimolar amounts of sodium nitrite
Source: Bayer AG Leverkusen

(17)

5.8 Toxicity to Reproduction

Type: Two generation study
Species: rat Sex: male/female
Strain: other: Slonaker-Addis
Route of admin.: oral feed
Exposure Period: see: type and remarks
Frequency of treatment: daily
Duration of test:

Doses: 0.1, 0.25 or 0.5 % = ca. 67, 167 or 333 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance: other TS: "virtually 100 % pure with a minimum purity of 99.9 %"
Remark: Post observation period: no data
Experimental design: the rats were assigned the diets when 5 w old, there being 12 females and 3 males on each dietary level; when the animals were 100 d old they were mated, 4 females and one male to a cage; once a week for 3 weeks the males were rotated among their 3 groups of females, after which time the males were removed and the females placed in individual cages; after all litters were weaned, the rats were remated; in addition, offspring from the first mating were mated once, in the same manner, for a second generation study
Result: the average size of the litters decreased as the concentration of dietary diphenylamine increased, with the anomalous exception of the numbers of pups born and weaned in the second generation whose mothers were fed the 0.1 % diet (however these rats grew to normal weight in 21 d);

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the food consumptions of the mothers were not measured, but the author assumes that less food was consumed by the gestating and lactating rats fed the 0.5 % diet, at least; the average weights at weaning were significantly less than their controls in but one group: the pups of the second generation, whose mothers were fed the 0.5 % diphenylamine concentration (in the authors opinion this fact casts reasonable doubt on any conclusion that this one instance of decreased weights was caused by diphenylamine alone)
Source: Bayer AG Leverkusen

(31) (94)

Type: other: modified Chernoff-Kavlock assay
Species: rat Sex: female
Strain: other: Alpk:AP
Route of admin.: gavage
Exposure Period: gestation days 7 to 17
Frequency of treatment: daily
Duration of test:
Doses: 1000 mg/kg bw/d
Control Group: yes
Method: other: see remarks
Year: GLP:
Test substance:
Remark: methods: maternal observations were restricted to body-weights on days 1, 7-17 and 22 of gestation; offspring ob-

servations were restricted to litter weights of live pups on days 1 and 5 post-partum and the numbers of live and dead pups on these days; no specific examination for malformations was conducted
Post observation period: 5 d

Result: reduced postnatal weight gain of the pups, litter sizes not affected, no reduction in postnatal survival of the pups

Source: Bayer AG Leverkusen

(108)

Type: other: see remarks
Species: rat Sex: male/female
Strain: Wistar
Route of admin.: oral feed
Exposure Period: 6 months
Frequency of treatment: daily
Duration of test:
Doses: 2 or 4 % (= ca. 1333 or 2667 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: 4 experimental animals per test group were used: 1 male, 2 pregnant females and 1 non-pregnant female
four experimental groups were used: group 1 received 2 % of diphenylamine in the diet; group 2 received 4 % of di-

phenylamine; group 3 received 2 % of diphenylamine and additionally 0.5 % of amino acids (D-L-methionine and L-cystine in equal shares); group 4 received 4 % of diphenylamine and 0.5 % of the amino acids mentioned above
Post observation period: no
test substance: technical diphenylamine containing 0.5 % aromatic amines (aniline and amino-4-diphenyl) as impurities
the pregnant rats received the diet beginning on the second or third day of gestation
type: the occurrence of abortions was observed

Result: all gestations ended in abortions prior to the second week of the experimental period

Source: Bayer AG Leverkusen

(75)

Type: other: see remarks
Species: rat Sex: female
Strain: Sprague-Dawley
Route of admin.: oral unspecified
Exposure Period: during the last 7 d of gestation (from 14 d gestation to term)
Frequency of

treatment: daily
Duration of test:
Doses: see remarks
Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: Post observation period: no
study design: two experimental groups were analyzed;
in group I, the pregnant rats were offered a mixture of either 1.5 or 2.5 % diphenylamine in rat chow (= ca. 1000 or 1667 mg/kg bw/d) for the last 7 d of gestation;
in group II, the following chemicals were fed by gastric tube to pregnant rats for 7 d prior to delivery: commercial diphenylamine or chromatographically purified diphenylamine (daily doses: 20 mg/animal) or three different trace impurities (contaminants E, F and G) that were detectable in commercial diphenylamine and that were identified in further analytical studies as N,N,N-triphenyl-p-phenylenediamine, o-cyclohexylaniline and p-cyclohexylaniline, respectively (daily doses: 50 ug/animal); all viable newborn rats were removed from the mothers shortly after birth and histologic kidney sections were prepared from the newborns and from the mother rats
type: in utero induction of cystic tubular lesions in kidneys of newborn rats
Result: the histology of the kidneys of mothers fed diphenylamine in both groups I and II was normal and no tubular dilatation or other abnormalities were observed;
feeding 2.5 % diphenylamine induced cystic changes in the proximal tubules of the newborn kidney; commercial diphenylamine and the contaminant E (each given by gastric tube) frequently induced moderate cystic changes in the

proximal tubules of the newborn rat; chromatographically pure diphenylamine did not result in significant cystic changes; the two other contaminants, labelled F and G, did not induce significant cystic tubular changes of the kidney in the newborn rat
Source: Bayer AG Leverkusen

(22) (23) (24) (82)

Type: other: see remarks
Species: rat Sex: male
Strain: no data
Route of admin.: oral unspecified
Exposure Period: no data
Frequency of treatment: daily
Duration of test:
Doses: 0.05, 0.5 or 5 mg/kg bw/d

Control Group: yes
Method:
Year: GLP:
Test substance:
Remark: a chronic experiment was performed (no further data concerning the exposure period)
Post observation period: no data
type: eventual gonadotropic effects of diphenylamine were investigated
Result: all dose levels: no gonadotropic effects
Source: Bayer AG Leverkusen

(62)

Type: other: see remarks
Species: guinea pig Sex: male/female
Strain: Hartley
Route of admin.: oral feed
Exposure Period: 6 months
Frequency of treatment: daily
Duration of test:
Doses: 2 or 4 % (= ca. 800 or 1600 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP:
Test substance: other TS: technical diphenylamine containing 0.5 % aromatic amines (aniline and amino-4-diphenyl) as impurities
Remark: 4 experimental animals per test group were used: 1 male, 2 pregnant females and 1 non-pregnant female
four experimental groups were used: group 1 received 2 % of diphenylamine in the diet; group 2 received 4 % of diphenylamine; group 3 received 2 % of diphenylamine and additionally 0.5 % of amino acids (D-L-methionine and L-cystine in equal shares); group 4 received 4 % of diphenylamine and 0.5 % of the amino acids mentioned above
Post observation period: no
the pregnant guinea pigs received the diet beginning on the second or third day of gestation

type: the occurrence of abortions was observed
Result: all gestations ended in abortions prior to the second week of the experimental period
Source: Bayer AG Leverkusen

(75)

5.9 Developmental Toxicity/Teratogenicity

Species: rabbit Sex: female
Strain: New Zealand white
Route of admin.: gavage

Exposure period: gestation days 7 to 19
Frequency of treatment: daily
Duration of test:
Doses: 33, 100 or 300 mg/kg bw/d
Control Group: yes
Method:
Year: GLP:
Test substance: other TS: purified diphenylamine (99.9 % purity)
Remark: on gestation day 29 the does were sacrificed and the foetuses were removed by caesarean section and examined for visceral and skeletal anomalies
Post observation period: no
Result: all dose groups: green discolouration of the urine (in particular at the 100 and 300 mg/kg bw dose levels); no increase in mortality; pregnancy rate unaffected; macroscopic findings unremarkable at terminal necropsy; litter size, litter weight, pre- and post-implantation loss and mean foetal weight not affected by diphenylamine; no compound-related fetal malformations or anomalies observable; incidence of visceral and skeletal anomalies unaffected by treatment at doses of diphenylamine up to and including 300 mg/kg bw 300 mg/kg bw: decrease in mean food consumption and reduction of mean body weight, no other signs of maternal toxicity
Source: Bayer AG Leverkusen

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