

I U C L I D

Data Set

Robust Summaries

Existing Chemical : ID: 10081-67-1
Memo : Crompton Corporation US HPV
CAS No. : 10081-67-1
EINECS Name : 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline
EC No. : 233-215-5
Molecular Formula : C30H31N

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2. Physico-Chemical Data

Id 10081-67-1
Date 06.01.2003

2.1 MELTING POINT

Value : 95 °C
Sublimation :
Method : other: no data
Year : 2001
GLP :
Test substance :
Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)
Trade name: Naugard 445
Source: Crompton Corporation

Reliability : (2) valid with restrictions
28.03.2003 (2)

2.2 BOILING POINT

Value : = 507.1 °C at
Decomposition :
Method : other: estimated using MPBPWIN v 1.40
Year : 2002
GLP :
Test substance : Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)

Remark : The safety data sheet for the substance reports an autoflammability temperature of 298°C, hence it will decompose before reaching its estimated boiling point.

Reliability : (2) valid with restrictions
23.12.2002 (2) (7)

2.4 VAPOUR PRESSURE

Value : = 6.67 hPa at 20 °C
Decomposition :
Method : other (measured): similar to OECD 104
Year : 1989
GLP : no
Test substance : Trade name: Naugard 445
Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)
Source: Uniroyal Chemical Company, Inc.
Purity: >99%
Lot No.: C-9-E29203

Remark : Measurements were made using the standard flask and manometer vapor pressure apparatus. After evacuating all vapor at -30°C, the sample was equilibrated at the various temperatures in a constant temperature bath.

Reliability : (2) valid with restrictions
28.03.2003 (5)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water

2. Physico-Chemical Data

Id 10081-67-1
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Log pow : = 8.51 at °C
pH value :
Method : other (calculated): KOWWIN v1.66
Year : 2002
GLP : no
Test substance : Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)
Reliability : (2) valid with restrictions
28.03.2003 (7)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 7 mg/l at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other
Year : 1986
GLP : no data
Test substance : Trade name: Naugard 455
Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)
Source: Uniroyal Chemical Company, Inc.
Purity: 98%
Lot No.: 6C302

Method : Excess substance added to 100 mL of water (HPLC grade) and sonicated for 4 hours, followed by standing for 1 hour to allow the solution to return to room temperature. The solution was filtered through Whatman #5 filter paper and diluted 1:1 with methanol prior to analysis using GC.

Result : Solvent: Solubility:
Water 7 mg/l
3% Acetic acid/water 6 mg/l
8% Ethanol/water 8.5 mg/l
Heptane 7400 mg/l

Reliability : (2) valid with restrictions
23.12.2002 (4)

3. Environmental Fate and Pathways

Id 10081-67-1
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3.1.1 PHOTODEGRADATION

Type : air
 Light source :
 Light spectrum : nm
 Relative intensity : based on intensity of sunlight
DIRECT PHOTOLYSIS
 Half-life t1/2 : .6 hour(s)
 Degradation : % after
 Quantum yield :
 Deg. product :
 Method : other (calculated): Estimation using AOPWIN v1.90
 Year :
 GLP :
 Test substance : Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)

 Test condition : 12 hr day, 1.5E6 OH/cm3
 Reliability : (2) valid with restrictions
 28.03.2003

(7)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
 Media :
 Air : % (Fugacity Model Level I)
 Water : % (Fugacity Model Level I)
 Soil : % (Fugacity Model Level I)
 Biota : % (Fugacity Model Level II/III)
 Soil : % (Fugacity Model Level II/III)
 Method : other: EPIWIN Level III Fugacity Model
 Year : 2003
 Test substance : Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)

 Test condition : Henry's Law Constant: 0.382 atm-m3/mole (Henrywin program)
 Vapor pressure: 5.01 mmHg (experimental)
 Log Kow: 8.51 (Kowwin program)
 Soil Koc: 1.33E+8 (calc by model)
 Melting point: 95 °C (experimental)

1000 kg/hr emissions to air, water and soil compartments.

	Mass Amount (percent)	Half-life (hr)	Emissions (kg/hr)
Air	0.0244	1.28	1000
Water	2.43	1.44E+3	1000
Soil	27.8	1.44E+3	1000
Sediment	69.7	5.76E+3	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.1E-12	985	18.2	32.8	0.606
Water	3.95E-9	87.2	181	2.91	6.04
Soil	3.41E-11	999	0	33.3	0
Sediment	3.85E-9	626	104	20.9	3.47

3. Environmental Fate and Pathways

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Persistence time: 2.49E+3 hr
Reaction time: 2.77E+3 hr
Advection time: 2.46E+4 hr
Percent reacted: 89.9
Percent advected: 10.1

Half-lives (hr), (based upon Biowin (ultimate) and Aopwin):

Air: 1.279
Water: 1440
Soil: 1440
Sediment: 5760
Biowin estimate: 1.788 (months)

Advection times (hr):

Air: 100
Water: 1000
Sediment: 5E+4

Reliability : (2) valid with restrictions
28.03.2003 (7)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :
Deg. product :
Method : other: Estimation using BIOWIN v4.00
Year : 2003
GLP :
Test substance : Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)

Result : MITI Linear Biodegradation Probability: -0.367
MITI Non-linear Biodegradation Probability: 0.0006

The chemical is predicted to be not readily biodegradable.
Reliability : (2) valid with restrictions
28.03.2003 (7)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type :
Species :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : .00023
Method : other: Estimation using Ecosar v0.99g
Year : 2003
GLP :
Test substance : Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)

Test condition : Log Kow: 8.51 (KOWWIN estimate)
MPt: 95°C (measured)
Water solubility: 7 mg/L (measured)

Reliability : (2) valid with restrictions
28.03.2003 (7)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit :
EC50 : .00038
Method : other: Estimation using Ecosar v0.99g
Year : 2003
GLP :
Test substance : Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)

Test condition : Log Kow: 8.51 (KOWWIN estimate)
MPt: 95°C (measured)
Water solubility: 7 mg/L (measured)

Reliability : (2) valid with restrictions
28.03.2003 (7)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species :
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : .000349
Method : other: Estimation using Ecosar v0.99g
Year : 2003
GLP :
Test substance : Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine (CAS No. 10081-67-1)

Test condition : Log Kow: 8.51 (KOWWIN estimate)
MPt: 95°C (measured)
Water solubility: 7 mg/L (measured)

Reliability : (2) valid with restrictions
28.03.2003 (7)

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : > 10000 mg/kg bw
Species : rat
Strain : other: Holtzman
Sex : male
Number of animals : 30
Vehicle : other: Corn oil
Doses : 215, 464, 1000, 2150, 4640 and 10000 mg/kg bw
Method : other: similar to OECD 401
Year : 1964
GLP : no
Test substance : Trade name: EPRA
 Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine
 Source: Naugatuck Chemical

Method : Dose: Single by gavage
 Post dose observation period: 14 days
 Weight range at start of study: 216-300 g
Result : No mortalities occurred at any dosage level tested.

The animals at each dosage level generally exhibited normal behaviour and appearance during the 14-d observation period.

Average body weight gains for the rats at each dosage level were within normal limits for rats of the age, sex and strain used in this study.

Gross autopsies performed on the rats at termination showed no significant gross pathology.

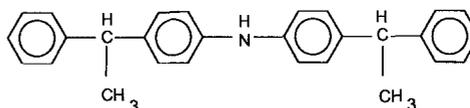
Conclusion : The acute oral LD50 of EPRA for male albino rats is >10000 mg/kg bw.

Reliability : (2) valid with restrictions
 No details of sample purity or Lot No.

06.01.2003

(3)

Type : LD50
Value : > 20000 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals : 25
Vehicle : other: corn oil
Doses : 2500, 5000, 10000, 20000, 40000 mg/kg
Method : other
Year : 1976
GLP : no
Test substance : Chemical name: Benzenamine, N-phenyl-, styrenated
 CAS #: 68442-68-2



Method : Dose: Single oral in 25% corn oil solution
 Post dose observation period: 14 days

5. Toxicity

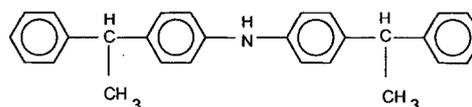
Id 10081-67-1

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The test parameters were based on a known and well established procedure for the time period.

Result : Two of the five animals died at the dosages of 20000 and 40000 mg/kg.
Conclusion : The LD50 of this analogue of the sponsored chemical was > 20000 mg/kg b.w.
Reliability : (2) valid with restrictions
06.01.2003 (1)

Type : LD50
Value : > 500 mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 10
Vehicle : other: corn oil
Doses : 500 mg/kg
Method : other: US Department of Transportation Regulations, 49CFR173.132 (1992)
Year : 1993
GLP : yes
Test substance : Chemical name: Benzenamine, N-phenyl-, styrenated
CAS #: 68442-68-2



Method : Dose: Single by gavage
Post dose observation period: 14 days

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.

Conclusion : The LD50 of this analogue of the sponsored chemical was > 500 mg/kg b.w.

Reliability : (2) valid with restrictions
06.01.2003 (1)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : .5 g
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 6
Vehicle : other: Corn oil
PDII :
Result : not irritating
Classification : not irritating
Method : other: similar to OECD 404
Year : 1964
GLP : no
Test substance : Trade name: EPRA
Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine
Source: Naugatuck Chemical

Result : EPRA produced no gross signs of dermal irritation on intact or abraded skin.

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Conclusion : Under the conditions of the test, EPRA is not a primary skin irritant.
Reliability : (2) valid with restrictions
No details of sample purity or Lot No.
23.12.2002 (3)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : 3 mg
Dose :
Exposure time : 72 hour(s)
Comment : not rinsed
Number of animals : 6
Vehicle : none
Result : not irritating
Classification : not irritating
Method : other
Year : 1964
GLP : no data
Test substance : Trade name: EPRA
Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine
Source: Naugatuck Chemical

Method : 3 mg of EPRA was applied to the right eye of each of six albino rabbits. The left eye was untreated and served as a control. Each rabbit was examined for eye irritative effects and for gross signs of systemic toxicity at intervals of 24, 48 and 72 hours after application.

Irritative effects observed in the eye were scored according to the Draize method.

Result : No gross signs of eye irritation were observed at any observation interval following application of EPRA to the eyes of albino rabbits.

All rabbits showed normal appearance throughout the study and there was no evidence of systemic toxicity from mucous membrane absorption.

Conclusion : EPRA produced no gross signs of eye irritation.
Reliability : (2) valid with restrictions
No details of sample purity or Lot No.

23.12.2002 (3)

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium: TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Test concentration : +/- S9: 0, 50, 150, 500, 1500 and 5000 µg/plate
Cytotoxic concentr. : >5000 µg/plate
Metabolic activation : with and without
Result : negative
Method : other: based on Ames, B.N. et al, Proc. Nat. Acad. Sci. USA (1973), 70, 2281
Year : 1985

- GLP** : yes
- Test substance** : Trade name: Naugard 445
Chemical name: 4,4'-Di-(alpha, alpha-dimethylbenzyl) diphenylamine
Purity: 98 %
- Method** : Metabolic activation: S9-mix, Rat liver cells, 0.5 ml, Aroclor induced
- Statistical Methods: no data
- Number of replicates: 3
- Positive controls:
- N-ethyl-N'-nitro-N-nitrosoguanidine (-S9, TA100 & TA1535)
9-aminoacridine (-S9, TA 1537)
2-nitrofluorene (-S9, TA1538 & TA98)
2-aminoanthracene (+S9, TA98, TA100, TA1535, TA1537 & TA1538)
- Negative control: Solvent vehicle
- Solvent: Dimethylsulfoxide
- Result** : The revertant colony counts for Naugard 445 obtained in the dose range finding test are shown in Table 1. Naugard 445 was not toxic towards the tester strains, therefore 5000 µg/plate was chosen as the top dose level in the mutation test.
- The mean number of revertant colonies, together with the individual plate counts for Naugard 445 obtained in the mutation test are shown in Table 2. Compound sterility and positive control mutability checks are shown in Table 3.
- No substantial increases in revertant colony numbers of any of the five tester strains were observed following treatment with Naugard 445 at any dose level, either in the presence or absence of metabolic activation (S9 mix).

Table 1. Dose range finding test on Naugard 445 - revertant colony counts obtained with *S. typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100

Dose level (ug/plate)	Metabolic activation	Strains of <i>S. typhimurium</i>				
		TA 1535	TA 1537	TA 1538	TA 98	TA 100
5000	-	12	10	9	12	120
500	-	4	14	11	15	112
50	-	6	12	4	14	90
5	-	7	12	13	21	90
Solvent	-	16	7	10	12	87
5000	+	9	12	18	23	132
500	+	5	22	11	20	122
50	+	10	19	8	18	99
5	+	8	17	23	14	98
Solvent	+	13	12	15	18	104

Table 2. Naugard 445 - revertant colony counts obtained per plate using *S. typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100

Strain	Dose level (ug/plate)	Without metabolic activation		With metabolic activation	
		Mean revertant colony counts	Individual revertant colony counts	Mean revertant colony counts	Individual revertant colony counts
TA 1535	5000	11	8, 12, 14	11	7, 11, 14
	1500	7	9, 9, 3	10	5, 12, 13
	500	14	16, 16, 9	9	11, 4, 11
	150	12	9, 13, 13	11	9, 9, 15
	50	14	23, 5, 13	9	5, 11, 12
	0	15	15, 15, 16	10	11, 4, 14
	Solvent	14	15, 11, 15	13	10, 15, 13
TA 1537	5000	13	17, 13, 9	19	15, 20, 21
	1500	19	18, 27, 11	14	10, 19, 14
	500	12	20, 9, 6	16	18, 20, 11
	150	16	19, 15, 15	17	15, 19, 18
	50	7	7, 10, 4	18	18, 14, 21
	0	11	12, 12, 10	12	14, 14, 8
	Solvent	8	8, 5, 10	18	21, 19, 14
TA 1538	5000	10	9, 12, 8	22	25, 19, 22
	1500	15	21, 11, 12	14	16, 18, 8
	500	9	13, 3, 12	17	10, 22, 18
	150	11	8, 16, 9	19	23, 17, 18
	50	8	11, 8, 6	16	17, 7, 23
	0	7	7, 4, 10	12	10, 7, 19
	Solvent	9	9, 8, 9	15	20, 12, 13
TA 98	5000	19	18, 18, 21	20	25, 14, 22
	1500	19	17, 20, 20	23	23, 22, 23
	500	15	14, 15, 17	21	28, 16, 20
	150	19	20, 20, 16	23	27, 20, 23
	50	18	14, 21, 19	17	14, 17, 21
	0	22	27, 20, 19	18	15, 21, 19
	Solvent	21	12, 27, 23	23	22, 21, 26
TA 100	5000	101	103, 99, 100	105	104, 97, 115
	1500	87	91, 102, 69	126	121, 121, 136
	500	114	116, 112, 114	130	128, 121, 142
	150	99	109, 83, 106	105	100, 102, 114
	50	105	91, 116, 107	134	127, 128, 146
	0	106	104, 109, 105	119	124, 119, 114
	Solvent	82	107, 67, 72	100	105, 104, 90

Table 3. Mutability and sterility tests with *S. typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 & TA 100

Strain	Compound	Dose level (ug)	Metabolic activation	Mean revertant colony counts	Individual revertant colony counts
TA 1535	N-ethyl-N'-nitro-N-nitrosoguanidine	5	-	220	199, 232, 229
TA 1537	9-aminoacridine	80	-	2175	2036, 2352, 2138
TA 1538	2-nitrofluorene	2	-	58	51, 76, 47
TA 98		1	-	72	68, 60, 89
TA 100	N-ethyl-N'-nitro-N-nitrosoguanidine	3	-	406	432, 407, 379
TA 1535	2-aminoanthracene	2	+	108	114, 105, 106
TA 1537		2	+	54	49, 53, 59
TA 1538		0.5	+	227	214, 255, 213
TA 98		0.5	+	121	126, 128, 110
TA 100		0.5	+	281	294, 293, 257
-	S-9 mix	500 ul		0	0
-	Naugard 445	5000		0	0

Conclusion

: It is concluded that no evidence of mutagenic potential of Naugard 445 was obtained in this bacterial test system at the dose levels used.

Reliability : (1) valid without restriction
24.12.2002 Study conducted following recognised test method under GLP. (6)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

9. References

Id 10081-67-1
Date 13.09.2002

- (1) American Chemistry Council, Rubber and Plastic Additives Panel, HPV Chemical Challenge Program Submission, Substituted Diphenylamines (DPA), December 2001
- (2) Crompton Corporation, Naugard 445 Safety Data Sheet, MSDS # C266001, Rev. 6, August 2001
- (3) Hill Top Research Institute, Inc., Acute oral, primary skin irritation and eye irritation studies on IVTI, XKIE, FFUU, EPRA and BUTAZATE. 1964.
- (4) In-house study conducted by Uniroyal Chemical Company, Inc.'s Chemical Characterization Laboratory, 1986
- (5) In-house study conducted by Uniroyal Chemical Company, Inc.'s Chemical Characterization Laboratory, 1989
- (6) Jones, E., Fenner, L.A., Thompson, A.L., Huntingdon Research Centre, Ames metabolic activation test to assess the potential mutagenic effect of Naugard 445, HRC Report No. URL 33/851340, 1985
- (7) US EPA, EPIWIN v3.10, EPI Suite Software, 2000