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2006 DEC 21 AM 7:26

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
Revision date:
Date of last Update: OCT-2006

Number of Pages: 8

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

Date: 02-NOV-2001

ID: 36878-20-3

2. Physico-chemical Data

2.1 Melting Point

Value: <0 °C

Decomposition: Yes [] No [] Ambiguous []

Sublimation: Yes [] No [] Ambiguous []

Method: [e.g. OECD, other

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

Remarks: Liquid at room temperature. This is a thick liquid made up of several components and is not meant to crystallize. The substance can be cooled to a glassy state or hard state but there will not be a point when that happens, like with a melting point. The 'melt point' is < 32F/0C.

Reference: Noveon Corporation (2006) Personal Communication; Flexsys (2006) Personal Communication

2.2 Boiling Point

*2.2 BOILING POINT

Value: 258 C

Pressure: 50 kPa

Decomposition: Yes [X] No [] Ambiguous []

Method: OECD 103

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

Remarks: The sample degraded before boiling at atmospheric pressure. Degradation was evidenced by an exothermic transition starting at ~260°C. When measured under pressure 50 kPa the boiling point measured 258°C.

Results:

Boiling Endotherm

Replicate	Sample Weight, mg	Ambient Pressure	Endotherm Peak °C
A	16.96	98.8 kPa	N/A
B	9.94	98.8 kPa	N/A
	Average =	N/A	N/A

Replicate	Sample Weight, mg	Vacuum	Endotherm Peak °C
A	10.98	50.27 kPa	259

Reliability: (2) Valid with Restrictions

Reference: Ciba (2006) THERMAL ANALYSIS LABORATORY REPORT.

2.4 Vapour Pressure

-

2.5 Partition Coefficient

-

2.6.1 Water Solubility

-

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Date: 02-NOV-2001

3. Environmental Fate and Pathways

ID: 36878-20-3

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
Control substance: 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 ± 1°C. 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

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Date: 02-NOV-2001

ID: 36878-20-3

3. Environmental Fate and Pathways

test substance for 14 days.

Test substance: Benzamine, ar-nonyl-N-(nonylphenyl)-

Reliability: (1) valid without restriction

02-NOV-2001

(1)

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Date: 02-NOV-2001

ID: 36878-20-3

4. Ecotoxicity

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 CaCO₃; Analysis - Water was free of measurable quantities of pesticides; Water chemistry in test: DO (% Saturation) - 92 to 104%; pH - 7.2 to 8.0 Test Temperature (°C) - 22 ± 1 Test 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)

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Date: 02-NOV-2001

4. Ecotoxicity

ID: 36878-20-3

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 (°C) - 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:
02-NOV-2001

(1) valid without restriction

(2)

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Date: 02-NOV-2001

4. Ecotoxicity

ID: 36878-20-3

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:
Flag:
02-NOV-2001

(1) valid without restriction
Critical study for SIDS endpoint

(3)

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Date: 02-NOV-2001
ID: 36878-20-3

5. Toxicity

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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Date: 02-NOV-2001

ID: 36878-20-3

6. References

(1) Biodegradability study of benzenamine, ar-nonyl-N-(nonylphenyl)- using batch processing respirometry test. Ricerca Inc., 19 Aug 1998.

(2) Acute toxicity of the water accommodated fraction (WAF) of benzenamine, ar-nonyl-N-(nonylphenyl)- to the mysid *Mysidopsis bahia*. EnviroSystems,, 04 October 1991.

(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.

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I U C L I D

Data Set

Existing Chemical : ID: 10081-67-1
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

Producer related part
Company : Epona Associates, LLC
Creation date : 14.07.2003

Substance related part
Company : Epona Associates, LLC
Creation date : 14.07.2003

Status :
Memo : RAPA

Printing date : 25.10.2006
Revision date :
Date of last update : 25.10.2006

Number of pages : 15

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type :
Physical status : solid
Purity :
Colour : white to off-white
Odour : characteristic

14.07.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

14.07.2003

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : = 98.5 °C
Sublimation :
Method :
Year : 2003
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : 98.5 deg C at STP
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
14.07.2003

(2)

2.2 BOILING POINT

Decomposition :
Method :
Year : 2006
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : The substance is a solid. Determination of the boiling point is not applicable.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
25.10.2006

(1)

2.3 DENSITY

Type : density
Value : = 1.14 g/cm³ at °C
Method :
Year : 2003
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
14.07.2003

(2)

2.3.1 GRANULOMETRY**2.4 VAPOUR PRESSURE****2.5 PARTITION COEFFICIENT****2.6.1 SOLUBILITY IN DIFFERENT MEDIA**

Solubility in : Water

2. Physico-Chemical Data

Id 10081-67-1
Date 25.10.2006

Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method :
Year : 2003
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Insoluble
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
14.07.2003 (2)

Solubility in : Organic Solvents
Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method :
Year : 2003
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Soluble
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
14.07.2003 (2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 276.7 °C
Type :
Method : other: Tag Closed Cup
Year : 2003
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
14.07.2003 (2)

2.8 AUTO FLAMMABILITY

Value : = 298 - °C at

2. Physico-Chemical Data

Id 10081-67-1
Date 25.10.2006

Method :
Year : 2003
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
14.07.2003

(2)

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

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

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

9. References

Id 10081-67-1
Date 25.10.2006

- (1) Chemtura Corporation (2006) Personal Communication
- (2) Crompton Material Safety Data Sheet (2003) Naugard 445.
Revision 1.1 05/28/2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

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REVISED OECD HPV FORM 1

SIDS DOSSIER ON THE HPV PHASE CHEMICAL Benzenamine, N-phenyl-, reaction products with isobutylene and 2, 4, 4-trimethylpentene CAS No. 184378-08-3

Sponsor Country :

DATE: ..October 2006

1. **GENERAL INFORMATION**

1.01 **SUBSTANCE INFORMATION**

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

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

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

†D. **CAS Descriptor** Benzenamine, N-phenyl-, reaction products with isobutylene and 2, 4, 4-trimethylpentene

E. **EINECS-Number** 270-128-1

F. **Molecular Formula**

*G. **Structural Formula**

H. **Substance Group**

I. **Substance Remark**

J. **Molecular Weight** 225-393

1.02 **OECD INFORMATION**

A. **Sponsor Country:** United States

B. **Lead Organisation:**

Name of Lead Organisation: Noveon, Inc.

Contact person: Robert K. Hinderer, Ph.D.

Address:

Street: 9911 Brecksville Rd.

Postal code: 44141-3247

Town: Cleveland, Ohio

Country: U.S.A.

Tel: (216)447-5181

Fax: (216)447-5760

C. **Name of responder**

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

Vanlube® 961

1.3 IMPURITIES

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

Remarks:

1.4 ADDITIVES

CAS No:
EINECS No:
Name:
Value:
Remarks:

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value: 280°K
Decomposition: Yes [] No [] Ambiguous []
Sublimation: Yes [] No [] Ambiguous []
Method: OECD 102
GLP: Yes [X] No [] ? []
Remarks: The sample was heated in a water bath starting at 19°C. At intervals of 3°C the jar containing the test sample was tilted to a horizontal position for a period of 5 seconds and was observed for signs of flow. The stationary point was determined to be 280°K and the pour point was determined to be 283°K.
Reliability: (1) Valid without Restrictions
Reference: O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

MELTING POINT

Value: 44-107°C
Decomposition: Yes No Ambiguous
Sublimation: Yes No Ambiguous
Method: Unknown
GLP: Yes No ?
Remarks: Range for major components; the melting point for the butylated/octylated component could not be determined because it is an oil.
Reference: BFGoodrich Laboratory (now Noveon, Inc.)

*2.2 BOILING POINT

Value: 549 +/- 0.5 K (=275 C)
Pressure: at 101.02 hPa
Decomposition: Yes No Ambiguous
Method: OECD 103
GLP: Yes No ?
Remarks: The boiling point was determined using a Mettler Toledo DSC12E calorimeter under static air atmosphere. The initial temperature was 20°C. The temperature was ramped at a rate of 20°C/min to a final temperature of 400°C. Because the material decomposed, no value for boiling temperature could be established. Therefore, the boiling temperature was estimated to be in the range of 575 to > 633 K using experimental databases for the diphenylamine impurity and an adaptation of the Stein and Brown method (Syracuse Research Corp., Inc. MPBP for Windows version 1.40, William Meylan, (1994-2000) to derive values for individual mono- and dialkyldiphenylamine components.
Reliability: (1) Valid without Restrictions
Reference: O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

BOILING POINT

Value: >200 °C
Pressure: at hPa
Decomposition: Yes No Ambiguous
Method: Unknown
GLP: Yes No ?
Remarks:
Reference: Noveon, Inc. MSDS

BOILING POINT

Value: Approx. 370 °C
Pressure: at hPa
Decomposition: Yes No Ambiguous
Method: EPIWIN
GLP: Yes No ?
Remarks: 326.04 to 431.62 for major components
Reference: EPIWIN

BOILING POINT

Value: 168 °C

Pressure: at hPa
 Decomposition: Yes [] No [**x**] Ambiguous []
 Method: measured
 GLP: Yes [] No [] ? []
 Remarks: Heating rate of 5 C per minute under a nitrogen atmosphere.
 Reference: Ciba (2006) Internal company data

†2.3 **DENSITY (relative density)**

Type: Bulk density []; Density [**X**]; Relative Density [] **Specific Gravity**
 Value: 977 kg/m³
 Temperature: 20.0 +/- 0.5 °C
 Method: OECD 109, 27 July 1995
 GLP: Yes [**X**] No [] ? []
 Remarks: A calibration was carried out by determining the mass of distilled water required to fill the glass pycnometer. The mass of the test material required to fill the pycnometer then was determined.
 Reliability: (1) Valid without Restrictions
 Reference: O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

DENSITY (relative density)

Type: Bulk density []; Density []; Relative Density [] **Specific Gravity**
 Value: Approx. 1
 Temperature: °C
 Method: Unknown
 GLP: Yes [] No [**X**] ? []
 Remarks:
 Reference: Noveon, Inc. MSDS

*2.4 **VAPOUR PRESSURE**

Value: 9.4x10⁻⁵ Pa
 Temperature: 25. °C
 Method: calculated []; measured [] OECD 104
 GLP: Yes [**X**] No [] ? []
 Remarks: The vapour pressure was determined using a vapour pressure balance with a sensitivity of approximately 0.1 µg. Temperature of the sample was controlled automatically and the temperature and mass readings were recorded automatically.
 Reliability: (1) Valid without Restrictions
 Reference: Tremain, S.P. (2002). Vanlube 961: Determination of Vapour Pressure, SafePharm Laboratories, Ltd.

VAPOUR PRESSURE

Value: 2x10-5 mmHg hPa
 Temperature: 25°C
 Method: calculated []; measured [] Unknown

GLP: Yes No ?
Remarks: CAS# 68411-46-1 has similar reaction products as CAS# 184378-08-3.
Uniroyal MSDS for CAS#68411-46-1 indicates negligible @20 degrees C .
Reference: CIBA MSDS for CAS# 68411-46-1

VAPOUR PRESSURE

Value: 1.14E-004 to 5.05E-008 hPa
Temperature: °C
Method: calculated ; measured EPIWIN
GLP: Yes No ?
Remarks: Range for major components
Reference: EPIWIN

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

Log Pow: 1.34×10^4 to $> 1.59 \times 10^6$, $\log_{10} P_{ow}$ 3.13 to >6.20
Temperature: °C
Method: calculated ; measured OECD 117
GLP: Yes No ?
Remarks: Following a preliminary test to approximate the solubilities of the test material in n-octanol and water, the test material (0.0276g) was diluted to 100 ml with acetonitrile. Solutions of reference standards also were prepared. The sample, thiourea, and referenced standard solutions were injected in duplicate in an HPLC , calibration curves were constructed, and retention times were determined. The capacity factors and $\log_{10} P_{ow}$ values then were calculated.
Reliability: (1) Valid without Restrictions
Reference: O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

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

Log Pow: $\gg 6$
Temperature: °C
Method: calculated ; measured Unknown
GLP: Yes No ?
Remarks: CAS# 68411-46-1 has similar reaction products as CAS# 184378-08-3.
Reference: CIBA MSDS for CAS# 68411-46-1

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

Log Pow: 5.2 to 10.82
Temperature: °C
Method: calculated ; measured EPIWIN
GLP: Yes No ?
Remarks: Range for major components
Reference: EPIWIN

*2.6 WATER SOLUBILITY

Value: 9.09 x10⁻² to 5.93x10⁻⁵
 Temperature: 20.0 +/- 0.5°C
 Description: Miscible []; Of very high solubility [];
 Of high solubility []; Soluble []; Slightly soluble [];
 Of low solubility []; Of very low solubility [X]; Not soluble []
 Method: OECD 105
 GLP: Yes [X] No [] ? []
 Remarks: An aliquote (0.5744g) of the test material was diluted to 500 ml with glass double distilled water. After shaking for 3¼ hours at 30°C and standing four 18 hours at 20°C, the solution was analysed by HPLC. The concentrations of the individual mono- and di-alkyldiphenylamine components and diphenylamine impurity ranged from 9.09 x10⁻² (DPA) to 5.93x10⁻⁵. These values are the means of three samples.
 Reliability: (1) Valid without Restrictions
 Reference: O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

WATER 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: Unknown
 GLP: Yes [] No [] ? []
 Remarks: CAS# 68411-46-1 has similar reaction products as CAS# 184378-08-3.
 Reference: CIBA MSDS. for CAS# 68411-46-1

WATER 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: EPIWIN
 GLP: Yes [] No [] ? []
 Remarks:
 Reference: EPIWIN

2.7 FLASH POINT

Value: >180 °C
 Type of test: Closed cup []; Open cup []; Other []
 Method: Pensky Martens.
 GLP: Yes [] No [X] ? []
 Remarks:
 Reference: BFGoodrich MSDS (Flash range)

2.8 AUTO FLAMMABILITY

Value: °C
Pressure: hPa
Method:
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:
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:
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:
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

Results:
Remarks:
Reference:

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

***3.1.1 PHOTODEGRADATION**

Type: Air []; Water []; Soil []; Other []
Light source: Sunlight []; Xenon lamp []; Other []
Light spectrum: nm
Relative intensity:
Spectrum of substance: 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): $\text{cm}^3/\text{molecule} \cdot \text{sec}$
Degradation:
Method: calculated []; measured [] 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:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
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:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
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 [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:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

3.6 BOD₅, COD OR RATIO BOD₅/COD

BOD₅

Method:
Concentration: related to COD [] ; DOC [] ; Test substance []
Value: mg O₂/l
GLP: Yes [] No [] ? []

COD

Method:
Value: mg O₂/g
GLP: Yes [] No [] ? []

Ratio BOD₅/COD:

Remarks:
Reference:

3.7 BIOACCUMULATION

Species:
Exposure period:
Temperature: °C
Concentration
BCF:
Elimination: Yes [] No [] ? []

Method:
Type of test: calculated []; measured []
 static []; semi-static []; flow-through []; other (*e.g. field test*) []
GLP: Yes [] No [] ? []
Test substance: purity:
Reference:

3.8 **ADDITIONAL REMARKS**

A. Sewage treatment

Results:
Remarks:
Reference:

B. Other information

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: LC₅₀ (24h) = mg/l
 LC₅₀ (48h) = mg/l
 LC₅₀ (72h) = mg/l
 LC₅₀ (96h) = mg/l
 NOEC = mg/l
 LOEC = mg/l
Analytical monitoring: Yes [] No [] ? []
Method:
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: EC₅₀ (24h) = mg/l
 EC₅₀ (48h) = mg/l
 EC_{xx} (..h) = mg/l

NOEC = mg/l
 Analytical monitoring: Yes [] No [] ? []
 Method:
 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: EC₅₀ (24h) = mg/l
 EC₅₀ (48h) = mg/l
 EC_{xx} (.h) = mg/l
 NOEC = mg/l
 Analytical monitoring: Yes [] No [] ? []
 Method:
 GLP: Yes [] No [] ? []
 Test substance: purity:
 Remarks:
 Reference:

***4.3 TOXICITY TO AQUATIC PLANTS**

Species:
 Endpoint: Biomass []; Growth rate []; Other []
 Exposure period:
 Results: EC₅₀ (h) = mg/l
 (*Endpoint*) EC_{xx} (h) = mg/l
 NOEC = mg/l
 LOEC = mg/l
 Analytical monitoring: Yes [] No [] ? []
 Method:
 open-system []; closed-system []
 GLP: Yes [] No [] ? []
 Test substance: purity:
 Remarks:
 Reference:

4.4 TOXICITY TO BACTERIA

Type: Aquatic []; Field []; Soil []; Other []
 Species:
 Exposure Period:
 Results: EC₅₀ (. . . h) = mg/l
 EC_{xx} (. . . h) = mg/l
 Analytical monitoring: Yes [] No [] ? []
 Method:
 GLP: Yes [] No [] ? []
 Test substance: purity:

Remarks:
Reference:

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

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: . EC₅₀ (..d) = mg/l
(Endpoint) EC_{xx} (..d) = mg/l
NOEC = mg/l
LOEC = mg/l

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

Method:

GLP: Yes [] No [] ? []

Test substance: purity:

Remarks:

Reference:

(*4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

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: EC₅₀ (..... h) = mg/l
(Endpoint) EC_{xx} (..... d) = mg/l
NOEC = mg/l
LOEC = mg/l

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

Method:

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: EC₅₀ (.....d) = mg/kg
 (Endpoint) EC₅₀ (.....d) = mg/kg
 EC_{xx} (.....d) = mg/kg
 NOEC = mg/kg
 LOEC = mg/kg

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

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)
 Species:
 Endpoint: Emergence []; Growth []; Other []
 Exposure period:
 Results: EC₅₀ and/or LC₅₀ (7d) = mg/l
 EC₅₀ and/or LC₅₀(14d) = mg/l
 EC_{xx} and/or LC_{xx} (xxd) = mg/l
 NOEC = mg/l
 LOEC = mg/l

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

(b)
 Species:
 Endpoint: Emergence []; Growth []; Other []
 Exposure period:
 Results: EC₅₀ and/or LC₅₀ (7d) = mg/l
 EC₅₀ and/or LC₅₀(14d) = mg/l
 EC_{xx} and/or LC_{xx} (xxd) = mg/l
 NOEC = mg/l
 LOEC = mg/l

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

(c)
 Species:
 Endpoint: Emergence []; Growth []; Other []
 Exposure period:
 Results: EC₅₀ and/or LC₅₀ (7d) = mg/l
 EC₅₀ and/or LC₅₀(14d) = mg/l
 EC_{xx} and/or LC_{xx} (xxd) = mg/l
 NOEC = mg/l

LOEC =mg/l

Method:

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)

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

Type: Animal []; Aquatic []; Plant []; Terrestrial []; Other []

Results:

Remarks:

Reference:

4.9 ADDITIONAL REMARKS

Results:

Remarks:

Reference:

5. TOXICITY

***5.1 ACUTE TOXICITY**

5.1.1 ACUTE ORAL TOXICITY

Type: LD₀ []; LD₁₀₀ []; LD₅₀ [**X**]; LD_{L0} []; Other []
Species/strain: Sprague-Dawley CD rats
Value: >2500 mg/kg b.w.:
Discriminating dose:
Method: OECD 423
GLP: Yes [**X**] No [] ? []
Test substance: Vanlube 961 purity: 99%
Remarks: The test material was administered by a single gavage dose as a solution in arachis oil. A group of three fasted females was treated with the test material at a dose of 2000 mg/kg b.w. After allowing a sufficient time to determine survival in the female, a group of three fasted males then was treated with the test material at a dose of 2000 mg/kg b.w. Animals were observed for deaths or signs of toxicity at ½, 1, 2, and 4 hours after dosing and then once daily for fourteen days. Body weights were determined prior to dosing and at seven and fourteen days post exposure. All animals were subject to a gross pathological examination at termination. No deaths, signs of toxicity, or abnormalities were observed. Body weight gains were normal. Based on the test procedure the LD₅₀ was estimated to be greater than 2500 mg/kg b.w.
Reliability: (1) Valid without Restrictions
Reference: Driscoll, R. (2002). Vanlube 961: Acute Oral Toxicity in the Rat – Acute Toxic Class Method, SafePharm Laboratories, Ltd.

5.1.2 ACUTE INHALATION TOXICITY

Type: LC₀ []; LC₁₀₀ []; LC₅₀ []; LCL₀ []; Other []
Species/strain:
Exposure time:
Value:
Method:
GLP: Yes [] No [] ? []
Test substance:, purity:
Remarks:
Reference:

5.1.3 ACUTE DERMAL TOXICITY

Type: LD₀ []; LD₁₀₀ []; LD₅₀ []; LD_{L0} []; Other []
Species/strain:
Value: mg/kg b.w.
Method:
GLP: Yes [] No [] ? []
Test substance:, purity:
Remarks:
Reference:

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

Type: LC₀ []; LC₁₀₀ []; LC₅₀ []; LCL₀ []; Other []
 LD₀ []; LD₁₀₀ []; LD₅₀ []; LDL₀ []; Other []

Species/strain:
 Route of Administration: i.m. []; i.p. []; i.v. []; infusion []; s.c. []; other []

Exposure time:
 Value:
 Method:
 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:
 Highly corrosive (causes severe burns) [];
 Corrosive (causes burns) []; Irritating []; Not irritating []

Method:
 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:
 Irritating []; Not irritating []; Risk of serious damage to eyes []

Method:
 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: Twenty test and ten control animals were used in this study. Based on the results of the sighting tests, the concentrations of the test material was selected as follows:

Intradermal induction – A row of three injections (0.1 ml each): a) Freund’s Complete Adjuvant/ water (1:1), b) 25% in arachis oil BP, and c) 25% in arachis oil BP in a 1:1 preparation of Freund’s Complete Adjuvant in water; sites were evaluated at 24 and 48 hrs. Control animals received a) Freund’s Complete Adjuvant/ water (1:1), b) arachis oil BP, and c) a 50% formulation of arachis oil BP in Freund’s Complete Adjuvant/ water 1:1 and evaluated as the same as the test material.

Topical induction – 7 days after the injections undiluted as supplied was applied to the same area on the clipped shoulder region and covered by an occlusive patch. After 48 hrs the patch was removed and the site was evaluated.

Topical Challenge – On Day 21 undiluted as supplied and 75% in arachis oil BP was applied to a clipped area and covered with an occlusive patch. After 24 hrs the patch was removed; skin reactions were evaluated at 24 and 48 hours.

The intradermal and topical induction doses were based on the highest concentration that caused only mild to moderate irritation and was well tolerated systemically. The highest non-irritating concentration and one lower concentration were selected for the topical challenge.

The test material produced 0% (0/20) sensitization rate and was classified as a non-sensitizer to the guinea pig skin.

Reliability: (1) Valid without Restrictions
 Reference: Safepharm Laboratories Limited, 1996

***5.4 REPEATED DOSE TOXICITY**

Type : Sub-acute
 Species : rat
 Sex : male/female
 Strain : Sprague-Dawley CrI:CD® (SD) IGS BR
 Route of admin. : gavage
 Exposure period : Males: 43 days; Females: up to 54 days
 Frequency of treatm. : daily
 Post exposure period : none
 Doses : 0, 5, 25 and 125 mg/kg/day
 Control group : yes, concurrent vehicle
 NOEL : 5 mg/kg bw
 Method : other: OECD Guideline 422
 Year : 2006
 GLP : yes
 Test substance : as prescribed by 1.1 - 1.4

Method : The test material was administered by gavage to three groups each of ten male and ten female Sprague-Dawley CrI:CD® (SD) IGS BR strain rats, for up to fifty-four consecutive days, at dose levels of 5, 25 and 125 mg/kg/day. A control group of ten males and ten females was dosed with vehicle alone (corn oil).

Clinical signs, behavioural assessments, bodyweight development, food and water consumption were monitored during the study. Haematology and blood chemistry were evaluated prior to mating on five selected males and females from each dose group.

Pairing of animals within each dose group was undertaken on a one male: one female basis on Day 15 of the study, to produce litters.

Extensive functional observations were performed on five selected parental males from each dose group after the completion of the mating phase, and for five selected parental females from each dose group on Day 4 *post partum*.

Males were terminated on Day 43, followed by the termination of all surviving females and offspring on Day 5 *post partum*. All animals were subjected to a gross necropsy examination and histopathological evaluation of selected tissues was performed.

Result : Mortality: No treatment-related deaths were detected.
 Clinical Observations: No clinically observable signs of toxicity were detected.
 Behavioural Assessments: No treatment-related effects were detected.
 Functional Performance Tests: No treatment-related effects were detected.
 Sensory reactivity Assessments: No treatment-related effects were detected.
 Bodyweights: No adverse effect on bodyweight was observed for males throughout the treatment period, or for females during the maturation or gestation, however, a slight reduction in bodyweight gain was observed for females treated with 125 mg/kg/day during lactation.
 Food Consumption: No adverse effect on dietary intake was detected for males throughout the treatment period, or for females during the maturation or gestation, however, a slight reduction in dietary intake was observed for females treated with 125 mg/kg/day during lactation.
 Water Consumption: No intergroup differences were detected.
 Haematology: Slightly elevated activated partial thromboplastin time was observed for animals of either sex treated with 125 mg/kg/day during the pre-mating and terminal assessments. Platelet count was also reduced at the high dose, however, this was only seen during the pre-mating assessment.
 Blood Chemistry: Animals of either sex showed a reduction in total plasma protein, albumin and the albumin/globulin ratio, together with elevated aspartate aminotransferase and alkaline phosphatase levels, with effects extending into the female 25 mg/kg/day dose group. No such effects were detected for males treated with 25 mg/kg/day or for animals of either sex treated with 5 mg/kg/day.
 Necropsy of Adults: Two males treated with 125 mg/kg/day displayed a pale liver. There were no other treatment-related macroscopic observations at terminal kill.
 Organ Weights: Males treated with 125 mg/kg/day displayed elevated liver

weights, both absolute and relative to terminal bodyweight. No such effects were detected for females or for animals of either sex treated with 25 or 5 mg/kg/day. Reduced spleen weights were also evident for females treated with 125 mg/kg/day.

Histopathology: Histopathological examinations revealed centrilobular hepatocyte enlargement of the liver for animals of either sex treated with 125 mg/kg/day. Females treated with 25 mg/kg/day were similarly effected.

Conclusion : The oral administration of CAS No 184378-08-3 to rats by gavage, at a maximum dose level of 125 mg/kg/day, resulted in treatment-related changes at 125 and 25 mg/kg/day. The hepatic changes observed were regarded as adaptive in nature, however, the changes in the haematological and biochemical parameters were considered to represent an adverse health effect. The 'No Observed Effect Level' (NOEL) for systemic toxicity was therefore considered to be 5 mg/kg/day.

Reliability : (1) valid without restriction

Reference : SafePharm Laboratories (2006) CAS No. 184378: Oral (Gavage) Combined Repeat Dose Toxicity Study with Reproduction/Developmental Toxicity Screening Test in the Rat. SPL Project Number 1666-080.

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: Bacterial reverse mutation assay

System of testing: *Salmonella typhimurium* strains TA1535, TA1537, TA102, TA98, TA100

Concentration: 0, 50, 150, 500, 1500, 5000 µg/plate

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

Results:

Cytotoxicity conc: With metabolic activation: None at concentrations tested.
Without metabolic activation: None at concentrations tested.

Precipitation conc: None observed.

Genotoxic effects: + ? -

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

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

Method: OECD 471

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

Test substance: Vanlube 961, purity: 99%

Remarks: The strains were obtained from the University of California. Overnight sub-cultures were prepared in nutrient broth and incubated at 37°C for approximately 10 hours. The test material was dissolved in DMSO. Vehicle and positive controls were tested in parallel with the test material. A solvent treatment group was the vehicle control and the positive controls were as follows: **without liver S-9 activation** N-ethyle-N'-nitro-N-nitrosoguanidine (3µg/plate for TA100; 5µg/plate for TA1535), 9-aminoacridine (80µg/plate for TA1537), Mitomycin C (0.5µg/plate for TA102), 4-nitroquinoline (0.2µg/plate for TA198) and **with liver S-9 activation** 2-aminoanthracene (1µg/plate for TA100, 2µg/plate for TA11535 and TA1537), Benzo(a)pyrene (5µg/plate for TA98), 1,8-dihydroxyanthraquinone (10µg/plate for TA102).

Based on the preliminary toxicity studies a first experiment was conducted. The test material was assayed in triplicate using the concentrations described above. The test material formulation (0.1 ml) was added to the agar plates with and without S-9. All plates were incubated at 37°C for 48 hours and then the frequency of revertant colonies was assessed. A second experiment was then conducted in the same manner as the first.

The assay was considered valid if all spontaneous revertants were in normal ranges, all tester strain characteristics were confirmed and all tester strain cultures were in the approximate range of 1 to 9.9×10^9 bacteria per ml.

The test material was considered positive if it induced a reproducible, dose-related and statistically significant increase in the revertant count in at least one strain of bacteria.

In both experiments the revertant counts at all concentrations for all strains, both with and without S-9, were comparable to the vehicle control. Also, all positive controls performed normally. Based on the absence of any significant increases in the frequency of revertant colonies, the test material was considered to be non-mutagenic under the conditions of the test.

Reliability: (1) Valid without Restrictions
Reference: Thompson, P.W. (2002). Vanlube 961: Reverse Mutation Assay "Ames Test" Using *Salmonella typhimurium*, SafePharm Laboratories, Ltd.

B. NON-BACTERIAL IN VITRO TEST

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

* 5.6 GENETIC TOXICITY IN VIVO

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

*5.8.1 **TOXICITY TO FERTILITY**

Type : One generation study
Species : rat
Sex : male/female
Strain : Sprague-Dawley CrI:CD® (SD) IGS BR
Route of admin. : gavage
Exposure period : Males: 43 days; Females: up to 54 days
Frequency of treatm. : daily
Premating exposure period
Male : 14 days
Female : 14 days
Duration of test : 14 days prior to mating, throughout mating and gestation and continuing through lactation day 3
No. of generation studies : 1
Doses : 0, 5, 25 and 125 mg/kg/day
Control group : yes, concurrent vehicle
NOAEL parental : 5 - mg/kg bw
NOAEL F1 offspring : 25 - mg/kg bw
Method : OECD Guide-line 422
Year : 2006
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method	: The test material was administered by gavage to three groups each of ten male and ten female Sprague-Dawley Crl:CD® (SD) IGS BR strain rats, for up to fifty-four consecutive days, at dose levels of 5, 25 and 125 mg/kg/day. A control group of ten males and ten females was dosed with vehicle alone (corn oil). Details of toxicity assessment are described in section 5.4.
	Pairing of animals within each dose group was undertaken on a one male:one female basis on Day 15 of the study, to produce litters. The presence of sperm within the vaginal smear and/or vaginal plug in situ was taken as positive evidence of mating.
	Pregnancy and parturition: The following was recorded for each female: i) Date of mating jj) Date and time of observed start of parturition iii) Date and time of observed completion of parturition iv) Duration of gestation
Result	: Reproductive Screening: Mating: There was no effect on mating or fertility, however, a shorter gestation length was observed for females treated with 125 mg/kg/day. Offspring Litter Size and Viability: Slightly lower viability indices were observed at 125 mg/kg/day. No intergroup differences were observed for litter size at birth or sex ratio. Slightly lower total litter weights were observed at 125 mg/kg/day.
Conclusion	: Treatment-related effects on reproduction were observed at 125 mg/kg/day, consisting of shorter gestation lengths and a higher incidence of offspring deaths. No such effects were detected at 25 mg/kg/day, therefore the 'No Observed Adverse Effect Level' (NOAEL) for reproductive toxicity was considered to be 25 mg/kg/day.
Reliability	: (1) valid without restriction
Reference	SafePharm Laboratories (2006) CAS No. 184378: Oral (Gavage) Combined Repeat Dose Toxicity Study with Reproduction/Developmental Toxicity Screening Test in the Rat. SPL Project Number 1666-080.

*5.8.2 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species	: rat
Sex	: male/female
Strain	: Sprague-Dawley Crl:CD® (SD) IGS BR
Route of admin.	: gavage
Exposure period	: Males: 43 days; Females: up to 54 days
Frequency of treatm.	: daily
Duration of test	: 14 days prior to mating, throughout mating and gestation and continuing through lactation day 3
Doses	: 0, 5, 25 and 125 mg/kg/day
Control group	: yes, concurrent vehicle
NOAEL maternal tox.	: 5 - mg/kg bw
NOAEL teratogen.	: 25 - mg/kg bw
Method	: other: OECD Guideline 422
Year	: 2006
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4

- Method** : The test material was administered by gavage to three groups each of ten male and ten female Sprague-Dawley CrI:CD® (SD) IGS BR strain rats, for up to fifty-four consecutive days, at dose levels of 5, 25 and 125 mg/kg/day. A control group of ten males and ten females was dosed with vehicle alone (corn oil). Details of toxicity assessment are described in section 5.4, and details of reproductive screening are described in section 5.8.1. During the lactation phase, daily clinical observations were performed on all surviving offspring, together with litter size and offspring weights and assessment of developmental landmarks.
- Result** : **Developmental Screening:**
Litter Observations: The number of interim deaths at 125 mg/kg/day was considerably higher than that observed for controls.
Offspring Viability: Slightly lower mean offspring weights were observed at 125 mg/kg/day.
Offspring Development: No treatment-related effects were detected.
Necropsy of Offspring: Interim death and terminal kill offspring did not show any abnormalities considered to be related to treatment.
- Reliability** : (1) valid without restriction
- Reference** SafePharm Laboratories (2006) CAS No. 184378: Oral (Gavage) Combined Repeat Dose Toxicity Study with Reproduction/Developmental Toxicity Screening Test in the Rat. SPL Project Number 1666-080.

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: (e.g. neurotoxicity, immunotoxicity, etc.)

Results:

Remarks:

Reference:

B. Toxicodynamics, toxicokinetics

Type:

Results:

Remarks:

References:

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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: October 2006

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

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

B. Name (IUPAC name)

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

†D. CAS Descriptor Benzenamine, N-phenyl-, reaction products with styrene and 2, 4, 4-trimethylpentene

E. EINECS-Number 272-940-1

F. Molecular Formula

***G. Structural Formula**

H. Substance Group

I. Substance Remark

J. Molecular Weight 225-633

1.02 OECD INFORMATION

A. Sponsor Country: United States

B. Lead Organisation:

Name of Lead Organisation: Noveon, Inc.

Contact person: Robert K. Hinderer, Ph.D.

Address:

Street: 9911 Brecksville Rd.

Postal code: 44141-3247

Town: Cleveland, Ohio

Country: U.S.A.

Tel: (216)447-5181

Fax: (216)447-5760

C. Name of responder

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 98%

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

1.3 IMPURITIES

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

CAS No:
EINECS No:
Name:
Value:
Remarks:

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value: <0 °C
Decomposition: Yes [] No [] Ambiguous []
Sublimation: Yes [] No [] Ambiguous []
Method: [e.g. OECD, other] .
GLP: Yes [] No [x] ? []

Remarks: Liquid at room temperature. This is a thick liquid made up of several components and is not meant to crystallize. The substance can be cooled to a glassy state or hard state but there will not be a point when that happens, like with a melting point. The 'melt point' is < 32F/0C.

Reference: Noveon Corporation (2006) Personal Communication; Flexsys (2006) Personal Communication

***2.2 BOILING POINT**

Value: >198 °C
Pressure: at hPa
Decomposition: Yes [] No [] Ambiguous []
Method
GLP: Yes [] No [] ? [x]
Remarks:
Reference: Noveon, Inc. MSDS

BOILING POINT

Value: 175 °C
Pressure: at hPa
Decomposition: Yes [] No [] Ambiguous []
Method: measured
GLP: Yes [] No [x] ? []
Remarks: Heating rate of 5 C per minute under nitrogen atmosphere
Reference: Ciba (2006) Internal company data

BOILING POINT

Value: 392.71 TO 663.07 °C
Pressure: at hPa
Decomposition: Yes [] No [] Ambiguous []
Method: EPIWIN
GLP: Yes [] No [] ? [x]
Remarks: Range for the components
Reference: EPIWIN

†2.3 DENSITY (relative density)

Type: Bulk density []; Density []; Relative Density [x] **Specific Gravity**
Value: 0.97-1.01
Temperature: °C
Method
GLP: Yes [] No [] ? []
Remarks:
Reference: Noveon, Inc. MSDS

***2.4 VAPOUR PRESSURE**

Value: 9.99E-007 to 1.9E-015 hPa
Temperature: °C
Method: calculated []; measured [] EPIWIN

GLP: Yes [] No [] ? []
Remarks: Range for components
Reference: EPIWIN

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

Log Pow: 5.2
Temperature: Room Temperature, 21 °C
Method: calculated []; measured [x]
OECD Section 1 N0. 107; EEC Annex V Test Guideline A.*, September 19, 1984
GLP: Yes [] No [x] ? []
Remarks: Concentrations of Vanlube SL-HP, extracted into water were measured by UV. Because the test material has a low solubility in water, accurate test concentrations are difficult to prepare. Thus the molar absorbtivity in water was assumed to be similar to that in n-octanol. The concentration of the test material in the octanol layer was approximately 0.8 molar. This concentration, higher than suggested in the guidelines, was necessary so that enough test material would be extracted into water (about 5×10^{-6} molar) to be detectable by UV. The change in concentration of the test material in the n-octanol before and after extraction is so small that the initial concentration of the test material is taken to be the concentration at equilibrium.

The molecular weight of monoctyl diphenylamine, 281, was taken as a representative MW of the test material.

The Log Pow was determined to be 5.2.
Reliability: (2) Valid with limitations
Flag: Critical study for SIDS endpoint
Reference: BFGoodrich Co., Brecksville R&D Center, November 28, 1990 (now Noveon, Inc.)

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

Log Pow: 5.45 to 15.13
Temperature: Room Temperature, 21 °C
Method: calculated []; measured [] EPIWIN
GLP: Yes [] No [] ? []
Remarks:
Reference: EPIWIN

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

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:
GLP: Yes [] No [] ? []
Remarks:
Reference: Noveon, Inc. 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: EPIWIN
GLP: Yes [] No [] ? []
Remarks: Range for components
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: EPIWIN

2.7 FLASH POINT (*liquids*)

Value: 180 °C
Type of test: Closed cup []; Open cup []; Other []
Method:
GLP: Yes [] No [] ? []
Remarks:
Reference: Noveon, Inc. MSDS

2.8 AUTO FLAMMABILITY (*solid/gases*)

Value: °C
Pressure: hPa
Method:
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:
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:
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:

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

Results:

Remarks:

Reference:

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air [x]; Water []; Soil []; Other []

Light source: Sunlight []; Xenon lamp []; Other []

Light spectrum: nm

Relative intensity:

Spectrum of substance: 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): $\text{cm}^3/\text{molecule}\cdot\text{sec}$
Degradation:
Method: calculated []; measured [] 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 $^{\circ}\text{C}$
Degradation: at pH at $^{\circ}\text{C}$ after
(exposure time)
Method:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

3.1.3 STABILITY IN SOIL

Type : Field trial []; Laboratory []; Other []
Radiolabel: Yes [] No [] ? []
Concentration:
Soil temperature: $^{\circ}\text{C}$
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:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
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 [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:
Reliability: (2) Valid with restrictions
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:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

3.6 BOD₅, COD OR RATIO BOD₅/COD

BOD₅

Method:
Concentration: related to COD []; DOC []; Test substance []
Value: mg O₂/l
GLP: Yes [] No [] ? []

COD

Method:
Value: mg O₂/g
GLP: Yes [] No [] ? []

Ratio BOD₅/COD:

Remarks:
Reference:

3.7 BIOACCUMULATION

Species:
Exposure period:
Temperature: °C
Concentration
BCF:
Elimination: Yes [] No [] ? []
Method:
Type of test: calculated []; measured []
static []; semi-static []; flow-through []; other (e.g. field test) []
GLP: Yes [] No [] ? []
Test substance: purity:
Reference:

3.8 ADDITIONAL REMARKS

A. Sewage treatment

Results:
Remarks:
Reference:

B. Other information

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: LC₅₀ (24h) = mg/l
LC₅₀ (48h) = mg/l
LC₅₀ (72h) = mg/l
LC₅₀ (96h) = mg/l
NOEC = mg/l
LOEC = mg/l

Analytical monitoring: Yes No ?

Method:

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: EC₅₀ (24h) = mg/l
EC₅₀ (48h) = mg/l
EC_{xx} (.h) = mg/l
NOEC = mg/l

Analytical monitoring: Yes No ?

Method: /

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: Mysid shrimp

Exposure period: 96 hr

Results: EC₅₀ (24h) = mg/l
 EC₅₀ (48h) = mg/l
 EC_{xx} (.96h) = 2.3 mg/l
 NOEC = <1.3 mg/l

Analytical monitoring: Yes No ?

Method: .OECD Guidelines 471 B14 in EC Directive 92/69/EEC

GLP: Yes No ?

Test substance: 100% active ingredient, purity:

Remarks: Solutions of the test material were prepared by dilution with sea water. After mixing and allowing undissolved material to settle, the water soluble fraction was added to two corresponding replicate test vessels. Two control vessels were established containing the same dilution water but no test material. The test concentrations 0, 1.3, 2.2, 3.6, 6, and 10 mg/l were selected based on preliminary test results. Mysids then were added to the test and control vessels. Test organisms were carefully transferred into the appropriate concentrations of newly prepared vessels at the 24, 48, and 72 hour observation periods. In life observations and water analyses were conducted at 0, 24, 48, 72 and 96 hours.

Following 96-hours of exposure, 60-100% mortality was observed in the three highest concentrations, and 25 and 40% mortality was observed in the two lowest concentrations. The 96-hour LC₅₀ was determined to be 2.3 mg/l (1.3-10 mg/l; 95% confidence limits. The 96-hour NOEC was < 1.3 mg/l.

Reliability: (1) Valid without restrictions

Reference: Springborn Laboratories, Inc. Report #89-11-3144 (January 10, 1990)

***4.3 TOXICITY TO AQUATIC PLANTS**

Species:

Endpoint: Biomass ; Growth rate ; Other

Exposure period:

Results: EC₅₀ (h) = mg/l
 (Endpoint) EC_{xx} (h) = mg/l
 NOEC = mg/l
 LOEC = mg/l

Analytical monitoring: Yes No ?

Method: open-system ; closed-system

GLP: Yes No ?

Test substance: purity:

Remarks:

Reference:

4.4 TOXICITY TO BACTERIA

Type: Aquatic ; Field ; Soil ; Other

Species:

Exposure Period:

Results: EC₅₀ (. . . h) = mg/l
 EC_{xx} (. . . h) = mg/l

Analytical monitoring: Yes No ?

Method:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

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: . EC₅₀ (..d) = mg/l
(Endpoint) EC_{xx} (..d) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes [] No [] ? []
Method:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

(*4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

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: EC₅₀ (..... h) = mg/l
(Endpoint) EC_{xx} (..... d) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes [] No [] ? []
Method:
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: EC₅₀ (.....d) = mg/kg
(Endpoint) EC₅₀ (.....d) = mg/kg
EC_{xx} (.....d) = mg/kg
NOEC = mg/kg
LOEC = mg/kg

Method:
 GLP: Yes No ?
 Test substance:, purity:
 Remarks:
 Reference:

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)
 Species:
 Endpoint: Emergence ; Growth ; Other
 Exposure period:
 Results: EC₅₀ and/or LC₅₀ (7d) = mg/l
 EC₅₀ and/or LC₅₀(14d) = mg/l
 EC_{xx} and/or LC_{xx} (xxd) = mg/l
 NOEC = mg/l
 LOEC = mg/l

Method:
 GLP: Yes No ?
 Test substance:, purity:
 Remarks:
 Reference:

(b)
 Species:
 Endpoint: Emergence ; Growth ; Other
 Exposure period:
 Results: EC₅₀ and/or LC₅₀ (7d) = mg/l
 EC₅₀ and/or LC₅₀(14d) = mg/l
 EC_{xx} and/or LC_{xx} (xxd) = mg/l
 NOEC = mg/l
 LOEC = mg/l

Method:
 GLP: Yes No ?
 Test substance:, purity:
 Remarks:
 Reference:

(c)
 Species:
 Endpoint: Emergence ; Growth ; Other
 Exposure period:
 Results: EC₅₀ and/or LC₅₀ (7d) = mg/l
 EC₅₀ and/or LC₅₀(14d) = mg/l
 EC_{xx} and/or LC_{xx} (xxd) = mg/l
 NOEC = mg/l
 LOEC = mg/l

Method:
 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)

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

Type: Animal []; Aquatic []; Plant []; Terrestrial []; Other []

Results:

Remarks:

Reference:

4.9 ADDITIONAL REMARKS

Results:

Remarks:

Reference:

5. TOXICITY

***5.1 ACUTE TOXICITY**

5.1.1 ACUTE ORAL TOXICITY

Type: LD₀ []; LD₁₀₀ []; LD₅₀ []; LDL₀ []; Other []
Species/strain:
Value: mg/kg b.w.:
Discriminating dose:
Method:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

5.1.2 ACUTE INHALATION TOXICITY

Type: LC₀ []; LC₁₀₀ []; LC₅₀ []; LCL₀ []; Other []
Species/strain:
Exposure time:
Value:
Method:
GLP: Yes [] No [] ? []
Test substance:, purity:
Remarks:
Reference:

5.1.3 ACUTE DERMAL TOXICITY

Type: LD₀ []; LD₁₀₀ []; LD₅₀ []; LDL₀ []; Other []
Species/strain:
Value: mg/kg b.w.
Method:
GLP: Yes [] No [] ? []
Test substance:, purity:
Remarks:
Reference:

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

Type: LC₀ []; LC₁₀₀ []; LC₅₀ []; LCL₀ []; Other []
LD₀ []; LD₁₀₀ []; LD₅₀ []; LDL₀ []; Other []
Species/strain:
Route of Administration: i.m. []; i.p. []; i.v. []; infusion []; s.c. []; other []
Exposure time:
Value:
Method:
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:
Highly corrosive (causes severe burns) [];
Corrosive (causes burns) []; Irritating []; Not irritating []
Method:
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:
Irritating []; Not irritating []; Risk of serious damage to eyes []
Method:
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: Sensitizing []; Not sensitizing [x]
Method: Shalanski Patch Test
GLP: Yes [] No [x] ? []
Test substance: BFGoodrich Material No. 2 (Stalite) , purity: Unknown
Remarks: 25 males and 25 females volunteers were used in this study. 13 of each sex were African Americans and 12 of each sex were Caucasians selected for considerable suntan to facilitate the assessment of depigmentation potential. The test material was applied to identical spots on the backs of the volunteers for 24-hours every other day for 15 applications. Two weeks after the induction period the sites were challenged with the test material for 24-hours. Reactions were evaluated when the patches were removed.

A minimal transitory reaction was noted in 3 males and 4 females; these were considered insignificant and minimal. No depigmentation was noted.

The material was considered not to be a primary irritant, fatiguing agent or sensitizer.
 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: The test material (see concentrations above) was administered to rats (25/sex/group) for 64 weeks. The animals were individually housed and quarantined for 11 days prior to the start of the study. The control group was fed animal chow without the test material. The test material was diluted with peanut oil and then added to the diets to product the desired concentrations. Hematologic evaluations were conducted on 5 rats/sex/group at the initiation of the test and at interval of 3 months throughout the study. Animals were observed for growth. Histopathological exams were conducted on 88 animals which died during the study (14) or were sacrificed at the end of the weeks 51, 56, and 58. Those animals that were sacrificed were representative of the groups with respect to sex and dietary level.

 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. The degenerative changes in the liver were described as diffuse cloudy swellings and fatty metamorphosis of the cytoplasm of the hepatocyte. 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 typhimurium*, 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: OECD 471 B14 in EC Directive 92/69/eec

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

Test substance: Vanlube® SL, purity: .98 %

Remarks: Remarks: The *S. typhimurium* strains were obtained from the University of California (Berkeley), and the *E. coli* strain was obtained from the British Industrial Biological Research Association. Overnight subcultures of the stock cultures were prepared in nutrient broth and incubated at 37°C for approximately 10 hours. The test material was dissolved in acetone to prepare the test concentrations noted above. Vehicle and positive controls were run in parallel with the test material. The positive controls were as follows:

Non-activation
TA100: N-ethy-N'-nitrosoquanidine (ENNG), 3 µg/plate
TA1535: ENNG, 5 µg/plate
TA1537: 9-aminoacridine, 80 µg/plate
TA98: 4-nitroquinoline-1-oxide, 0.2 µg/plate
WP2uvrA: ENNG, 2 µg/plate

Activation (10% liver S9)
TA100: 2-Aminoanthracene (2AA), 1 µg/plate
TA1535: 2AA, 2 µg/plate
TA1537: 2AA, 2 µg/plate
TA98: 2AA, 0.5 µg/plate
WP2uvrA: 2AA, 10 µg/plate

A preliminary toxicity study was conducted to select the appropriate dose levels. Five doses of the test material and the vehicle control (acetone) were tested in duplicate. In addition, 0.1 ml of the maximum concentration of the test material and 2 ml of the molten medium were overlaid onto an agar plate. After 48 hours incubation at 37°C the plates were assessed for revertant colonies.

Two experiments were conducted to assess reproducibility. A substance was considered positive if it induce a dose-related and statistically significant increase in mutation rate (at least twice the spontaneous reversion rate) in one or more strains with or without activation. (Note: In the event of two equivocal experiments a third experiment may be used.) To be considered negative the number of induced revertants compared to

the spontaneous revertants should be less than two fold at each dose level employed, the intervals of which should be between two and five fold and extend to the limits imposed by toxicity, solubility or up to the maximum recommended dose of 5000 ug/plate. (Note: In this case the limiting factor was the maximum recommended dose.)

No toxicity was observed to any of the strains. Precipitates were observed at 1500 ug/plate and 5000 ug/plate but did not interfere with scoring. No significant increase in the frequency of revertant colonies was recorded in any strain with or without activation, and the responses of the positive controls were satisfactory.

Reliability: (1) Valid without limitations
Reference: Safepharm Laboratories Limited, Project No. 860/032, 17 December 1997

B. NON-BACTERIAL IN VITRO TEST

Type:
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:
GLP: Yes No ?
Test substance: , purity:
Remarks:
Reference:

* 5.6 GENETIC TOXICITY IN VIVO

Type:
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:
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:
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:
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: (e.g. neurotoxicity, immunotoxicity, etc.)

Results:
Remarks:
Reference:

B. Toxicodynamics, toxicokinetics

Type:
Results:
Remarks:
References:

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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: . . . October 2006

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

- *A. Cast number** 68608-77-5
- B. Name (IUPAC name)**
- *C. Name (OECD name)**
- †D. CAS Descriptor** Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives
- E. EINECS-Number** 271-800-7
- F. Molecular Formula**
- *G. Structural Formula**
- H. Substance Group**
- I. Substance Remark**
- J. Molecular Weight** 225-479

1.02 OECD INFORMATION

- A. Sponsor Country:** United States
- B. Lead Organisation:**

Name of Lead Organisation: Noveon, Inc.

Contact person: Robert K. Hinderer, Ph.D

Address:

Street: 9911 Brecksville Rd.

Postal code: 44141-3247

Town: Cleveland

Country: U.S.A.

Tel: (216)447-5181

Fax: (216)447-5760

- 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 100 %

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

1.3 IMPURITIES

CAS No:

EINECS No:

Name:

Value:

Remarks:

1.4 ADDITIVES

CAS No:

EINECS No:

Name:

Value:

Remarks:

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value: <0 °C
Decomposition: Yes No Ambiguous
Sublimation: Yes No Ambiguous
Method: *[e.g. OECD, other]* .
GLP: Yes No ?
Remarks: Liquid at room temperature. This is a thick liquid made up of several components and is not meant to crystallize. The substance can be cooled to a glassy state or hard state but there will not be a point when that happens, like with a melting point. The 'melt point' is < 32F/0C.
Reference: Noveon Corporation (2006) Personal Communication; Flexsys (2006) Personal Communication

*2.2 BOILING POINT

Value: 221 °C
Pressure: at hPa
Decomposition: Yes No Ambiguous
Method: measured
GLP: Yes No ?
Remarks: Heating rate of 5C per minute under a nitrogen atmosphere
Reference: Ciba (2006) Internal company data

Value: 443.18 – 547.61 °C
Pressure: at hPa
Decomposition: Yes No Ambiguous
Method: 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)

Type: Bulk density ; Density ; Relative Density **Specific Gravity**
Value: 0.915-0.955
Temperature: °C
Method:
GLP: Yes No ?
Remarks: Specific Gravity
Reference: Noveon, Inc. MSDS 2001

*2.4 VAPOUR PRESSURE

Value: 2.35E-008 to 9.18E-012 hPa
Temperature: 25 °C
Method: calculated ; measured EPIWIN
GLP: Yes No ?
Remarks: Based on the two reaction products that are 90+% of all reaction products...
Reference: EPIWIN

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

Log Pow: 9.84
Temperature: °C
Method: calculated [x]; measured [] EPIWIN.
GLP: Yes [] No [] ? []
Remarks: Based on the two reaction products that are 90+% of all reaction products..
Reference: EPIWIN

***2.6 WATER SOLUBILITY**

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: 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:
GLP: Yes [] No [] ? []
Remarks:
Reference: Noveon, Inc. MSDS 2001

B. pH Value, pKa Value

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

2.7 FLASH POINT (*liquids*)

Value: 213 °C
Type of test: Closed cup []; Open cup []; Other []
Method:
GLP: Yes [] No [] ? []
Remarks:
Reference:

2.8 AUTO FLAMMABILITY (*solid/gases*)

Value: °C
Pressure: hPa
Method:
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:
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:
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:

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

Results:

Remarks:

Reference:

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air ; Water [] ; Soil [] ; Other []
Light source: Sunlight [] ; Xenon lamp [] ; Other []
Light spectrum: nm
Relative intensity:
Spectrum of substance: 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): cm³/molecule*sec
Degradation:
Method: calculated [] ; measured [] 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:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
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:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
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 [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
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

3.6 BOD₅, COD OR RATIO BOD₅/COD

BOD₅

Method:

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

Value: mg O₂/l

GLP: Yes [] No [] ? []

COD

Method:

Value: mg O₂/g

GLP: Yes [] No [] ? []

Ratio BOD₅/COD:

Remarks:

Reference:

3.7 BIOACCUMULATION

Species:

Exposure period:

Temperature: °C

Concentration:

BCF:

Elimination: Yes [] No [] ? []

Method:

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

Results:

Remarks:

Reference:

B. Other information

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: LC₅₀ (24h) = mg/l
LC₅₀ (48h) = mg/l
LC₅₀ (72h) = mg/l
LC₅₀ (96h) = mg/l
NOEC = mg/l
LOEC = mg/l

Analytical monitoring: Yes No ?

Method:

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: EC₅₀ (24h) = mg/l
EC₅₀ (48h) = mg/l
EC_{xx} (.h) = mg/l
NOEC = mg/l

Analytical monitoring: Yes No ?

Method:

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: EC₅₀ (24h) = mg/l
EC₅₀ (48h) = mg/l
EC_{xx} (.h) = mg/l
NOEC = mg/l

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

Method:

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: EC₅₀ (.....h) = mg/l
EC_{xx} (.....h) = mg/l
NOEC = mg/l
LOEC = mg/l

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

Method: open-system []; closed-system []

GLP: Yes [] No [] ? []

Test substance: . purity:

Remarks:

Reference:

4.4 TOXICITY TO BACTERIA

Type: Aquatic []; Field []; Soil []; Other []
Species:
Exposure Period:
Results: $EC_{50} (\dots h) = \dots \text{mg/l}$
 $EC_{xx} (\dots h) = \dots \text{mg/l}$
Analytical monitoring: Yes [] No [] ? []
Method:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

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: $EC_{50} (..d) = \dots \text{mg/l}$
 $EC_{xx} (..d) = \dots \text{mg/l}$
NOEC = $\dots \text{mg/l}$
LOEC = $\dots \text{mg/l}$
Analytical monitoring: Yes [] No [] ? []
Method:
GLP: Yes [] No [] ? []
Test substance: purity:
Remarks:
Reference:

(*4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

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
 EC_{xx} (..... d) = mg/l
NOEC = mg/l
LOEC = mg/l

Analytical monitoring: Yes No ?

Method:

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
 EC_{50} (..... d) = mg/kg
 EC_{xx} (..... d) = mg/kg
NOEC = mg/kg
LOEC = mg/kg

Method:

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:
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:
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:
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)

Results: Substance:
Species or ecosystem studied:
Effects monitored:
Results:
Chemical analysis:
Remarks:
Reference:

4.8 BIOTRANSFORMATION AND KINETICS

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

4.9 ADDITIONAL REMARKS

Results:
Remarks:
Reference:

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD₀ []; LD₁₀₀ []; LD₅₀ [**x**]; LDL₀ []; Other []
Species/strain: Rat/Charles River strain (COBS)
Value: >34,600 mg/kg b.w.:
Discriminating dose:
Method:
GLP: Yes [] No [**x**] ? []
Test substance:), Goodrite® 3185 , purity: 100%
Remarks: Based on range finding data groups of rats (2/sex/group) were administered 10,250, 15,380, 23,070, or 34,600 mg/kg via oral gavage. Animals were observed for toxic signs; body weights were recorded at the beginning of the study and at the end of the 14-day observation period. No mortality was observed at any of the doses.
Reliability: (2) Reliable with restrictions.
Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor (now Noveon, Inc.)

5.1.2 ACUTE INHALATION TOXICITY

Type: LC₀ []; LC₁₀₀ []; LC₅₀ []; LCL₀ []; Other [**x**]
Species/strain: Rats/Sprague-Dawley
Exposure time: 4 hrs
Value:
Method:
GLP: Yes [] No [**x**] ? []
Test substance: .), Goodrite® 3185 , purity: 100%..
Remarks: A groups of rats (5/sex/group) was exposed to the test material via inhalation exposure. Animals were observed for toxic signs; body weights were recorded at the beginning of the study and at the end of the 14-day observation period. Because of the materials low volatility, no weight loss of the test material was noted. No deaths were observed.
Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor (now Noveon, Inc.)

5.1.3 ACUTE DERMAL TOXICITY

Type: LD₀ []; LD₁₀₀ []; LD₅₀ []; LDL₀ []; Other []
Species/strain: Rabbit/New Zealand
Value: >3,000 mg/kg b.w.
Method:
GLP: Yes [] No [**x**] ? []
Test substance: . Goodrite® 3185 purity: 100%
Remarks: The test material was applied to a shaved area on the backs of four rabbits and then covered with an impervious plastic sheeting. After 4 hours the test material was removed, and the sites were examined for local reactions. Animals were observed for toxic signs; body weights were recorded at the beginning of the study and at the end of the 14-day observation period. No

mortality was observed at any of the doses. Skin reactions were limited to mild erythema, desquamation, and edema. Only barely perceptible to slight erythema and desquamation were present at day 14.

Reliability: (2) Reliable with restrictions.

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

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

Type: LC₀ []; LC₁₀₀ []; LC₅₀ []; LCL₀ []; Other []
LD₀ []; LD₁₀₀ []; LD₅₀ []; LDL₀ []; Other []

Species/strain:

Route of Administration: i.m. []; i.p. []; i.v. []; infusion []; s.c. []; other []

Exposure time:

Value:

Method:

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:

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:

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

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

Remarks: The eye irritation study was patterned after the Draize method (1944). Only conjunctival reactions were observed and only at the 1 hour observation.
Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor (now Noveon, Inc.)

5.3 SKIN SENSITISATION

Type:
Species/strain:
Results: Sensitizing []; Not sensitizing []; Ambiguous []
Classification: Sensitizing []; Not sensitizing []
Method:
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: [] 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 []; 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 [] No [] ? []

Test substance: Vanlube NA, purity: ..100 %

Remarks: The *S. typhimurium* strains were obtained from the University of California (Berkeley), and the *E. coli* strain was obtained from the British Industrial Biological Research Association. Overnight subcultures of the stock cultures were prepared in nutrient broth and incubated at 37°C for approximately 10 hours. The test material was dissolved in acetone to prepare the test concentrations noted above. Vehicle and positive controls were run in parallel with the test material. The positive controls were as follows:

Non-activation
TA100: N-ethy-N'-nitrosoquanidine (ENNG), 3 µg/plate
TA1535: ENNG, 5 µg/plate
TA1537: 9-aminoacridine, 5 µg/plate
TA98: 4-nitroquinoline-1-oxide, 0.2 µg/plate
WP2uvrA: ENNG, 2 µg/plate

Activation (10% liver S9)
TA100: 2-Aminoantracene (2AA), 1 µg/plate
TA1535: 2AA, 2 µg/plate
TA1537: 2AA, 2 µg/plate
TA98: 2AA, 0.5 µg/plate
WP2uvrA: 2AA, 10 µg/plate

A preliminary toxicity study was conducted to select the appropriate dose levels. Five doses of the test material and the vehicle control (acetone) were tested in duplicate. In addition, 0.1 ml of the maximum concentration of the test material and 2 ml of the molten medium were overlaid onto an agar plate. After 48 hours incubation at 37°C the plates were assessed for revertant colonies.

Two experiments were conducted to assess reproducibility. A substance was considered positive if it induce a dose-related and statistically significant increase in mutation rate (at least twice the spontaneous reversion rate) in one or more strains with or without activation. (Note: In the event of two equivocal experiments a third experiment may be used.) To be considered negative the number of induced revertants compared to the spontaneous revertants should be less than two fold at each dose level employed, the intervals of which should be between two and five fold and extend to the

limits imposed by toxicity, solubility or up to the maximum recommended dose of 5000 ug/plate. (Note: In this case the limiting factor was the maximum recommended dose.)

No toxicity was observed to any of the strains. Precipitates were observed at 1500 ug/plate and 5000 ug/plate but did not interfere with scoring. No significant increase in the frequency of revertant colonies was recorded in any strain with or without activation, and the responses of the positive controls were satisfactory.

Reliability: (1) Reliable without limitations

Reference: Safepharm Laboratories Project No. 860/026, 21 May 1997, Sponsor R.T. Vanderbilt Co., Inc.

Flag: Critical study for SIDS endpoint and acceptable for assessment

Type: Bacterial reverse mutation assay

System of testing: *Salmonella typhimurium* strains TA-1535, TA-1537, TA-1538, TA-98, TA-100

Concentration: 0.5 to 5,000 ug/plate

Cytotoxic Conc.: With metabolic activation: 0.5 to 100 ug/plate (little to no toxicity)

Without metabolic activation: 0.5 to 100 ug/plate (little to no toxicity)

Metabolic activation: with and without

Result: negative

Method: other: according to other: according to Ames et al (1975)

Mutation Res. 31:347-364; McCann et al. (1975) Proc. Nat. Acad. Sci. 72:5135-5139

Year: 1979 GLP: no data

Test substance: Good-rite® NEPA, purity: ..100 %

Remark: The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations.

Salmonella typhimurium strains TA-1535, TA-1537, TA-1538, TA-98 and TA-100 were obtained from Dr. Bruce Ames. All indicator strains were kept at 4°C on minimal medium plates supplemented with a trace of biotin and an excess of histidine (Ames, 1980). In addition, the plates with the plasmid-carrying *Salmonella* strains (TA-98 and TA-100) were supplemented with 26µg/ml of ampicillin to ensure stable maintenance of the plasmid pKM101. “

The bacterial strains were cultured at 37°C in Oxid Media #2 (nutrient broth), and Vogel Bonner Medium E with 2% glucose was used as the selective medium (Vogel and Bonner, 1956). The overlay agar was prepared according to the method of Ames et al (1975). S-9 liver homogenates, which were prepared from Aroclor 1254-induced and noninduced adult Sprague-Dawley male rats as described by Ames et al (1975, were prepared from Binetics Laboratory Products, Litton Bionetics, Inc. An S-9 mix was prepared by adding the following ingredients per milliliter of mix: 4 µmoles NADP (sodium salt), 5 µmoles D-glucose-6-phosphate, 8 µmoles MgCL₂, 33 µmoles KCL, 100 µmoles sodium phosphate buffer (pH 7.4), and 100 µl of rat liver S-9 fraction.

All tests were based on the methods of Ames et al (1975). Test compounds were dissolved in dimethylsulfoxide (DMSO). Solvent and positive controls are

summarized as follows: Positive controls for the non-activation assays were 1 ug/plate sodium azide for TA-1535 and TA-100, 50 ug/plate 9-aminoacridine for TA-1537, 10 µg 2-nitrofluorene for TA-1538 and TA-98. The positive control used for the activation assays was 2.5 ug/plate 2-anthramine.) "The highest dose was established as one which produced some toxicity.

Criteria which were used to determine whether a chemical was mutagenic were: 1) an increase in revertants in strains TA-1535, TA-1537, TA-1538 of three times the solvent control; 2) an increase in revertants in strains TA-98 and TA-100 of twice the solvent control; 3) reproducibility; and 4) a dose-related response, and a consistent pattern of response between strains derived from the same parental strain

Signed QA assurance statement provided

Reliability: (2) Reliable with restrictions. Meets generally accepted scientific standards, well documented.
Reference: Litton Bionetics, Inc. Project No. 20988, September 1979, Sponsor BFGoodrich (now Noveon, Inc.).

B. NON-BACTERIAL IN VITRO TEST

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

*** 5.6 GENETIC TOXICITY IN VIVO**

Type:
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:
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:
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:

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:
Results:
Remarks:
Reference:

B. Toxicodynamics, toxicokinetics

Type:
Results:
Remarks:
References:

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I U C L I D

D a t a S e t

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

Type: Lead organization
Name: American Chemistry Council (formerly Chemical Manufacturers Association) Rubber and Plastics Additives (RAPA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States
Phone: 703-741-5600
Facsimile: 703-741-6091

Type: cooperating company
Name: Bayer Polymers LLC
Country: United States

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Country: United States

Type: cooperating company
Name: Crompton Corporation
Country: United States

Type: cooperating company
Name: Flexsys America L.P.
Country: United States

Type: cooperating company
Name: Noveon, Inc (formerly BF Goodrich)
Country: United States

1. General Information

Type: cooperating company
Name: R.T. Vanderbilt Company, Inc.
Country: United States

Type: cooperating company
Name: The Goodyear Tire & Rubber Company
Country: United States

Type: cooperating company
Name: Eliokem Inc.
Country: United States

Type: cooperating company
Name: The Lubrizol Corporation
Country: United States

Type: cooperating company
Name: UOP, LLC.
Country: United States

Number of Pages: 15

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential

Printing date: 25-Feb-03
Revision date:
Date of last Update: 10-NOV-06

date: 25-Feb-03

1. General Information

Substance ID: 68442-68-2

1.1 General Substance Information

Substance type: organic
Physical status: liquid
Purity: > 98 % w/w
Result: Molecular weight: 320
25-Feb-03

1.2 Synonyms

Mixed styrenated diphenylamines
N-Phenyl benzenamine, styrenated
p-Oriented styrenated diphenylamines
Styrene, reaction product with diphenylamine
SDPA
Styrenated diphenylamine
Styrenated N-phenylbenzenamine
Vulkanox DDA
WINGSTAY 29
WINGSTAY 29 POWDERED
WINGSTAY 29E
WTR Number 8b

1.3 Impurities

CAS-No: 122-39-4
EINECS-No: 204-539-4
CAS Name: Benzenamine, N-phenyl-
EINECS-Name: diphenylamine
Contents: < .5 % w/w

1.4 Additives

CAS-No: 63231-67-1
CAS Name: Silica gel
EINECS-Name: Siica, hydrated amorphous
Contents: 30 % w/w
Remark: It is also sold as a powder that consists of 70% styrenated diphenylamine and 30% inert carrier. (7)

CAS-No: 112926-00-8
CAS Name: Silica gel, pptd., cryst.-free (DSL, PICCS, ASIA-PAC) Gel de silice precipitee, sans cristaux (French) (DSL) Silica gel, precipitated,

REVISED November 10, 2006
crystalline free (AICS) Synthetic amorphous silica, pptd. (ECL) AMORPHOUS
PRECIPITATED SILICA (PICCS) PRECIPITATED SILICA (PICCS) SILICA
GEL, PPTD. CRYST-FREE (PICCS) SYNTHETIC CRYSTALLINE-FREE SILICA GEL (PICCS)
SILICON DIOXIDE (PICCS) SILICA, HYDRATED AMORPHOUS (PICCS) SILICA GEL,
PRECIPITATED, CRYSTAL-FREE (PICCS) SILICA GEL (PICCS)

ECL Serial No.

KE-32733

Contents:

30 % w/w

Remark:

It is also sold as a powder that consists of 70% styrenated
diphenylamine and 30% inert carrier.

2. Physico-chemical Data

date: 26-Feb-03
Substance ID: 68442-68-2**2.1 Melting Point**

Value: ca. 6 degree C
Method: other
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Remark: Solidifying point
Reliability: (4) not assignable (8)

2.2 Boiling Point

Value: > 300 degree C at 1013 hPa
Method: other
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Remark: Actual method is unknown
Reliability: (4) not assignable (8)

2.3 Density

Type: density
Value: ca. 1.1 g/cm³ at 20 degree C
Method: other
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Reliability: (4) not assignable (8)

Type:
Value:
Method: other: ASTM D-891
Year: 1994
GLP: no data
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: Specific Gravity is 1.08-1.10
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP,
the test parameters used were based on a known and well
established procedure. (12)

2.4 Vapour Pressure

Value: < 100 hPa at 50 degree C
Method: other (measured)
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Reliability: (4) not assignable

(8)

2.5 Partition Coefficient

log Pow: 4.64 at 22 degree C
Method: other (measured)
Year: 1990
GLP: yes
Test substance: Vulkanox DDA
Reliability: (1) valid without restriction

(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
Test substance: Vulkanox DDA
Reliability: (1) valid without restriction

Value: See Results
Qualitative:
Method: OECD Guideline 105 for Testing of Chemicals (1995), EC Directive 92/69 Method A.6 (1992), column elution method
Year: 1990
GLP: yes
Test substance: Wingstay 29
Result: The water solubility of the components of the test item Wingstay 29 was determined to be:
 20.6 µg/L for p-SDPA
 < 58.8 µg/L (< LOQ) for p,p'-diSDPA
 < 27.6 µg/L (< LOQ) for o,p,p'-triSDPA
 at 20 °C and a pH value of 7.

Remark: CAS 68442-68-2 is defined as Benzenamine, N-phenyl-, styrenated. This is a reaction product which contains different components as mono, di and tri substituted material. Water solubility for Wingstay 29, CAS number 68442-68-2, has been measured for each major component mono, di and tri substituted.

Reliability: (1) valid without restriction

(16)

2.7 Flash Point

Value: > 100 degree C
Type: open cup
Method: other
Year: 1994
GLP: no data
Remark: Actual method is unknown

Value: 270 degree C
Type:
Method: other
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Reliability: (4) not assignable

(8)

date: 25-Feb-03

3. Environmental Fate and Pathways

Substance ID: 68442-68-2

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: Vulkanox DDA
Test substance: Batch No. C 40021 f 28.09.86
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP,
the test parameters used were based on a known and well
established procedure.

(1)

3.6 BOD5, COD or BOD5/COD Ratio

Method: other
Method: other
Test substance: Vulkanox DDA
Remark: ThOD: 2882 mg/g
Reliability: (4) not assignable

(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
Remark: Test substance dispersed in water by means of an Ultra-Turrax
Test substance: Vulkanox DDA
Test substance: Batch No. C 40021 of 28.08.86
Reliability: (2) valid with restrictions
 Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

(1)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: > 10000
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: 1986 **GLP:** no
Remark: Direct weight
Test substance: Vulkanox DDA
Test substance: Batch No. C 40021 of 28.09.86
Reliability: (2) valid with restrictions
 Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

(1)

date: 25-Feb-03

Substance ID: 68442-68-2

5. Toxicity

5.1 Acute Toxicity**5.1.1 Acute Oral Toxicity**

Type: LD50
Species: rat
Sex: no data
Number of Animals: 25
Vehicle: other: corn oil
Value: > 20000 mg/kg bw
Method: other
Year: 1976 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)

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 probably not conducted to GLP, the test parameters used were based on a known and well established procedure for the time period.

(5)

Type: LD50
Species: rat
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: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Method: Five (5) male and five (5) female young adult rats 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

(9)

date: 25-Feb-03

Substance ID: 68442-68-2

5. Toxicity

Type: LD50
 Species: rat
 Sex:
 Number of
 Animals: Unknown
 Vehicle:
 Value: > 5000 mg/kg bw
 Method: other
 Year: 1994 GLP: no data
 Test substance: Vulkanox DDA
 Reliability: (4) not assignable

(8)

5.1.3 Acute Dermal Toxicity

Type: LD50
 Species: rabbit
 Sex:
 Number of
 Animals: 5
 Vehicle:
 Value: > 10000 mg/kg bw
 Method: other
 Year: 1976 GLP: no
 Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
 Remark: No animals died after administration of 10000 mg/kg
 Reliability: (2) valid with restrictions
 Although this study was probably not conducted to GLP,
 the test parameters used were based on a known and well
 established procedure for the time period.

(3)

5.2 Corrosiveness and Irritation**5.2.1 Skin Irritation**

Species: rabbit
 Concentration:
 Exposure:
 Exposure Time:
 Number of
 Animals: Unknown
 PDII:
 Result: slightly irritating
 EC classificat.: not irritating
 Method: other
 Year: 1976 GLP: no
 Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
 Remark: Primary Skin Irritation. Was originally classified as
 non-irritating; however, according to current
 classifications, it would be a mild irritant. The result
 was 0.46.
 Reliability: (2) valid with restrictions
 Although this study was probably not conducted to GLP,
 the test parameters used were based on a known and well
 established procedure for the time period.

(2)

5. Toxicity

date: 25-Feb-03
 Substance ID: 68442-68-2

Species: rabbit
 Concentration:

Exposure:
 Exposure Time:
 Number of

Animals: Unknown

PDII:
 Result: not irritating
 EC classificat.: not irritating
 Method: other
 Year: 1994

GLP: no data

date: 25-Feb-03

Test substance: Vulkanox DDA
 Reliability: (4) not assignable

(8)

5.2.2 Eye Irritation

Species: rabbit
 Concentration:

Dose:
 Exposure Time:
 Comment:

Number of
 Animals: 6

Result: slightly irritating
 EC classificat.: not irritating
 Method: other
 Year: 1976

GLP: no

Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)

Remark: Standard protocol of the times for eye irritation. Mild irritant when not followed by wash. Six young adult albino rabbits, three with and three without a wash. Observations were made at 24, 48, and 72 hours and at 7 days.

Reliability: (2) valid with restrictions
 Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure for the time period.

(4)

Species: rabbit
 Concentration:

Dose:
 Exposure Time:
 Comment:

Number of
 Animals:

Result: not irritating
 EC classificat.: not irritating
 Method: other
 Year: 1994

GLP: no data

Test substance: Vulkanox DDA
 Reliability: (4) not assignable

(8)

5.4 Repeated Dose Toxicity

Type : Sub-acute
 Species : rat
 Sex : male/female
 Strain : Sprague-Dawley Crl:CD® (SD) IGS BR
 Route of admin. : gavage
 Exposure period : Males: 43 days; Females: up to 54 days
 Frequency of treatm. : daily
 Post exposure period : none
 Doses : 0, 50, 250 and 600 mg/kg/day
 Control group : yes, concurrent vehicle
 NOAEL : 600 mg/kg bw
 Method : other: OECD Guideline 422
 Year : 2006
 GLP : yes
 Test substance : as prescribed by 1.1 - 1.4

Method : The test material was administered by gavage to three groups each of ten male and ten female Sprague-Dawley Crl:CD® (SD) IGS BR strain rats, for up to fifty-four consecutive days, at dose levels of 50, 250 and 600 mg/kg/day. A control group of ten males and ten females was dosed with vehicle alone (corn oil).

Clinical signs, behavioural assessments, bodyweight development, food and water consumption were monitored during the study. Haematology and blood chemistry were evaluated prior to mating on five selected males and females from each dose group.

Pairing of animals within each dose group was undertaken on a one male: one female basis on Day 15 of the study, to produce litters.

Extensive functional observations were performed on five selected parental males from each dose group after the completion of the mating phase, and for five selected parental females from each dose group on Day 4 *post partum*.

Males were terminated on Day 43, followed by the termination of all surviving females and offspring on Day 5 *post partum*. All animals were subjected to a gross necropsy examination and histopathological evaluation of selected tissues was performed.

Result : Mortality: No treatment-related deaths were detected.
 Clinical Observations: No clinically observable signs of toxicity were detected.
 Behavioural Assessments: No treatment-related effects were detected.
 Functional Performance Tests: No treatment-related effects were detected.
 Sensory reactivity Assessments: No treatment-related effects were detected.
 Bodyweights: No adverse effect on bodyweight was observed for males throughout the treatment period, or for females during the maturation, gestation or lactation phases of the study.
 Food Consumption: No adverse effect on dietary intake was detected for males throughout the treatment period, or for females during the maturation, gestation or lactation phases of the study.
 Water Consumption: No overt intergroup differences were detected.

Haematology: No treatment-related changes were detected prior to mating.

Blood Chemistry Elevated alkaline phosphatase levels were detected for males treated with 600 mg/kg/day. Males treated with 600 and 250 mg/kg/day also showed reduced cholesterol levels. No such effects were detected for females treated with 600 or 250 mg/kg/day or for animals of either sex treated with 50 mg/kg/day.

Necropsy of Adults: No treatment-related macroscopic abnormalities were detected for the interim death female or for the remaining animals at terminal kill.

Organ Weights: Elevated liver and adrenal weights, both absolute and relative to terminal bodyweights, were detected for animals of either sex treated with 600 mg/kg/day.

Histopathology: Histopathological examination of adult tissue revealed the following treatment-related changes: Liver: Centrilobular hepatocyte enlargement was observed for animals of either sex treated with 600 and 250 mg/g/day, with the effect extending into the female 50 mg/kg/day dose group.

Thyroid glands: Follicular cell hypertrophy was observed for males treated with 600 and probably also at 250 mg/kg/day. No such effects were detected for females at these dose levels, or for animals of either sex treated with 50 mg/kg/day.

Conclusion : The oral administration of CAS No 68442-68-2 to rats by gavage, at dose levels of 600, 250 and 50 mg/kg/day, resulted in treatment-related effects at all dose levels. These effects however, were considered entirely adaptive in nature, therefore the 'No Observed Adverse Effect Level' (NOAEL) was considered to be 600 mg/kg/day.

Reliability : (1) valid without restriction

(15)

5.5 Genetic Toxicity 'in Vitro'

Type: 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

Metabolic activation: with and without

Result: negative

Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella typhimurium Reverse Mutation Assay"

Year: 2001 **GLP:** yes

Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)

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.

Positive controls were 2-nitrofluorene (TA98 without metabolic activation); sodium azide (TA100 and TA1535 without metabolic activation); IRC-191 (TA1537 without metabolic activation); 4-nitroquinoline-N-oxide (WP2uvrA without metabolic activation); benzo[a]byrene (TA98 with metabolic activation); and 2-Aminoanthracene (TA100, TA1535, TA1537, and WP2uvrA with metabolic activation).

Based on results of a range-finding study with Salmonella typhimurium (tester strain 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

date: 25-Feb-03

Substance ID: 68442-68-2

5. Toxicity

Type: Ames test
System of testing: Salmonella typhimurium Strains TA-98, 100, 1535, and 1537
Concentration: 1, 10, 100, and 1000 micrograms/l
Metabolic activation: with and without
Result: negative
Method: other
Year: 1980 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: Test compound was evaluated for genetic activity in the Ames test with and without the addition of mammalian metabolic activation. Negative and positive controls were run concurrent with the assay. No remark was made regarding which positive control was used with which strain. No remark whether positive controls were duplicate or triplicate.

Positive Controls: without activation - 2-nitrofluorene, sodium azide, quinacrine mustard
with activation 2-aminofluorene, 2-aminoanthracene,
dimethylbenz(a)anthracene

Negative Control: DMSO

Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP,
the test parameters used were based on a known and well
established procedure.

(13)

Type: Ames test
System of testing: Salmonella typhimurium Strains TA-98, 100, 1535, and 1537
Concentration: 10, 100, and 2000 micrograms/l
Metabolic activation: with and without
Result: negative
Method: other
Year: 1982 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: Test compound was evaluated for genetic activity in the Ames test with and without the addition of mammalian metabolic activation. Negative and positive controls were run concurrent with the assay. No remark was made regarding which positive control was used with which strain. No remark whether positive controls were duplicate or triplicate.

Positive Controls: without activation - 2-nitrofluorene, sodium azide, quinacrine mustard
with activation 2-aminofluorene, 2-aminoanthracene,
dimethylbenz(a)anthracene

Negative Control: DMSO

Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP,
the test parameters used were based on a known and well
established procedure.

(14)

5. Toxicity

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

Metabolic activation: with and without

Result: negative

Method: other

Year: 1981 **GLP:** no

Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)

Positive Controls: with activation - Tris(2,3 dibromopropyl)phosphate
without activation - Ethyl Methanesulfonate

Negative Control: Chloramphenicol

Remark: A test for the ability of the chemical to damage cellular DNA in the E coli Pol A1- Liquid Suspension Assay. Negative and positive controls were run concurrent with the assay.

Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure. (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: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)

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.

5. Toxicity

Statistical analyses were performed using Analysis of Variance and Dunnett's t-test.

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

(6)

5.8.1 Toxicity to Fertility

Type : One generation study
Species : rat
Sex : male/female
Strain : Sprague-Dawley Crl:CD® (SD) IGS BR
Route of admin. : gavage
Exposure period : Males: 43 days; Females: up to 54 days
Frequency of treatm. : daily
Premating exposure period
Male : 14 days
Female : 14 days
Duration of test : 14 days prior to mating, throughout mating and gestation and continuing through lactation day 3
No. of generation studies : 1
Doses : 0, 50, 250 and 600 mg/kg/day
Control group : yes, concurrent vehicle
NOAEL parental : 250 - mg/kg bw
NOAEL F1 offspring : - mg/kg bw
Method : OECD Guide-line 422
Year : 2006
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : The test material was administered by gavage to three groups each of ten male and ten female Sprague-Dawley Crl:CD® (SD) IGS BR strain rats, for up to fifty-four consecutive days, at dose levels of 50, 250 and 600 mg/kg/day. A control group of ten males and ten females was dosed with vehicle alone (corn oil). Details of toxicity assessment are described in section 5.4.

Pairing of animals within each dose group was undertaken on a one male:one female basis on Day 15 of the study, to produce litters. The presence of sperm within the vaginal smear and/or vaginal plug *in situ* was taken as positive evidence of mating.

Pregnancy and parturition: The following was recorded

for each female:

- i) Date of mating
- jj) Date and time of observed start of parturition
- iii) Date and time of observed completion of parturition
- iv) Duration of gestation

Result : Reproductive Screening:
Mating: No adverse effects on mating performance, fertility or gestation were detected.
Offspring Litter Size and Viability: Females treated with 600 mg/kg/day showed a higher percentage of pre-implantation losses in comparison to controls, resulting in the birth of less offspring per litter and lower total litter weights at this dose level.

Conclusion : Treatment-related effects on reproduction were observed at 600 mg/kg/day. These were confined to an increase in pre-implantation losses, resulting in lower offspring numbers at this dose level. The NOAEL for reproductive toxicity was therefore considered to be 250 mg/kg/day.

Reliability : (1) valid without restriction

(15)

5.8.2 Developmental Toxicity/Teratogenicity

Species : rat
Sex : male/female
Strain : Sprague-Dawley Crl:CD® (SD) IGS BR
Route of admin. : gavage
Exposure period : Males: 43 days; Females: up to 54 days
Frequency of treatm. : daily
Duration of test : 14 days prior to mating, throughout mating and gestation and continuing through lactation day 3
Doses : 0, 50, 250 and 600 mg/kg/day
Control group : yes, concurrent vehicle
NOAEL maternal tox. : 250 - mg/kg bw
NOAEL teratogen. : 250 - mg/kg bw
Method : other: OECD Guideline 422
Year : 2006
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : The test material was administered by gavage to three groups each of ten male and ten female Sprague-Dawley Crl:CD® (SD) IGS BR strain rats, for up to fifty-four consecutive days, at dose levels of 50, 250 and 600 mg/kg/day. A control group of ten males and ten females was dosed with vehicle alone (corn oil). Details of toxicity assessment are described in section 5.4, and details of reproductive screening are described in section 5.8.1. During the lactation phase, daily clinical observations were performed on all surviving offspring, together with litter size and offspring weights and assessment of developmental landmarks.

Result : Developmental Screening:
Litter Observations: There were no clinical signs to suggest an effect of treatment.
Offspring Viability: Mean offspring weights for treated animals were comparable to controls.
Offspring Development: Offspring from the 600 mg/kg/day dose group showed less successful completion of surface righting assessments. There were no treatment-related differences in pinna unfolding.
Necropsy of Offspring: No treatment-related macroscopic abnormalities were detected for the interim death offspring or for the remaining offspring at terminal

Reliability

kill.
: (1) valid without restriction

(15)

- (1) Bayer AG Data
- (2) Food and Drug Research Laboratories, Inc., Primary Skin Irritation Study with Rabbits, Laboratory Report No. 2688b to The Goodyear Tire & Rubber Company, 1976
- (3) Food and Drug Research Laboratories, Inc., Acute Dermal Toxicity in Rabbits, Laboratory Report No. 2688b to The Goodyear Tire & Rubber Company, 1976
- (4) Food and Drug Research Laboratories, Inc., Rabbit Eye Irritation Study, 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 #; 21054-0-4550ECD, Covance Laboratories (Vienna, Virginia), 1/19/01
- (7) It is also sold as a powder that consists of 70% styrenated diphenylamine and 30 % inert carrier.
- (8) Material Safety Data Sheet, Bayer AG, 1994
- (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 #: 21054-0-4090ECD, Covance Laboratories (Vienna, Virginia), 02/06/01
- (11) The Goodyear Tire & Rubber Company, E. coli Pol A1- Liquid Suspension Assay on WINGSTAY 29, 1981.
- (12) The Goodyear Tire & Rubber Company, Material Safety Data Sheet, 1994
- (13) The Goodyear Tire & Rubber Company, Mutagenicity Evaluation of WINGSTAY 29, 1980.
- (14) The Goodyear Tire & Rubber Company, Mutagenicity Evaluation of WINGSTAY 29, Laboratory Report No. 82-1-1, 1982.
- (15) SafePharm Laboratories (2006) CAS No. 68442-68-2: Oral (Gavage) Combined Repeat Dose Toxicity Study with Reproduction/Developmental Toxicity Screening Test in the Rat. SPL Project Number 1666-038.
- (16) DR.U.NOACK-LABORATORIEN, Käthe-Paulus-Str. 1, D-31157 Sarstedt, Germany under Laboratory Project ID: Project-No. 050601EM.

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Final Submission under the HPV Challenge Program for the Substituted Diphenylamines Category

CAS Nos. 68411-46-1, 68442-68-2, 184378-08-3, 101-67-7, 10081-67-1
36878-20-3, 68608-77-5 and 68921-45-9

Rubber and Plastic Additives Panel
American Chemistry Council
Revised November 2006

List of Member Companies in the Rubber and Plastic Additives Panel

The Rubber and Plastic Additives (RAPA) Panel of the American Chemistry Council (ACC) includes the following member companies: Alco Chemical Corporation; Bayer Polymers LLC.; Ciba Specialty Chemicals Corporation; Chemtura Corporation (formerly Crompton Corporation); Eliokem, Inc.; Flexsys America L.P.; The Goodyear Tire & Rubber Company; The Lubrizol Corporation; Noveon, Inc.; and R.T. Vanderbilt Company, Inc.

Executive Summary

The ACC's RAPA Panel, and its member companies, hereby submit the final category documentation for the Substituted Diphenylamines category of chemicals under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program. This submission is the finalization of the Substituted Diphenylamines category documents submitted on December 18, 2001 and August 5, 2003. In revising these documents, comments received from EPA (dated November 27, 2002) and Environmental Defense (dated May 15, 2003) have been considered, and all proposed testing has been completed and summarized.

As discussed in the report that follows, Substituted Diphenylamines, which are used as antidegradants in rubber, foamed polymers and high-temperature functional fluids (lubricants, gear oils, hydraulic fluids), are defined as amines with various substitutions. Their use in these applications requires stability at high temperatures, low biodegradation, low water solubility and low vapor pressure.

In consideration of animal welfare concerns to minimize the use of animals in the testing of chemicals, the Panel has conducted a thorough literature search for all available data, published and unpublished. It has also performed an analysis of the adequacy of the existing data. Further, it developed a scientifically supportable category of related chemicals and used structure-activity relationship information to address certain data requirements.

Substituted Diphenylamines Category

Relying on several factors specified in EPA's guidance document on "Development of Chemical Categories in the HPV Challenge Program," in which use of chemical categories is encouraged, the following closely related chemicals constitute a chemical category:

Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)
Benzenamine, N-phenyl-, styrenated (68442-68-2)
Benzenamine, N-phenyl- (184378-08-3)¹
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)

Structural Similarity. A key factor supporting the classification of these chemicals as a category is their structural similarity (see Figure 1). All share a common starting material; Diphenylamine (Benzenamine, N-phenyl-, CAS# 122-39-4), a common synthetic pathway, and all compounds in this category are diamines with various substitutions.

Similarity of Physicochemical Properties. The similarity of the physicochemical properties of these materials parallels their structural similarity. All are off-white to light brown solids or viscous liquids intended for use as antioxidants in finished rubber articles or as antidegradant additives that extend the useful life of heavy-duty industrial functional fluids used in high-speed, high-temperature and/or high-load applications. As a class, these amine-based antidegradant compounds are less migratory (more polymer-bound) and less staining than the Substituted p-Phenylenediamine antidegradants. The use of these materials requires that they be stable under high temperatures. Their low volatility is due to their low vapor pressure, highly viscous or solid form. The existing information for these materials indicates that they have low water solubility and high flash points.

Fate and Transport Characteristics. Members of this category have been shown to be not readily biodegradable, so additional testing is not needed. The lack of water solubility of the members of this category makes hydrolysis testing unnecessary. Adequate information regarding photodegradation is available for meeting HPV Program requirements; therefore, additional data collection efforts are not necessary. These materials have been shown not to partition to water or air if released into the environment due to their low water solubility and low vapor pressure.

Toxicological Similarity. Review of existing published and unpublished test data for Substituted Diphenylamines shows the aquatic and mammalian toxicity among the materials within this category are similar.

Aquatic Toxicology. With increasing molecular weight, the toxicity to aquatic organisms decreases. These materials have high estimated log Kow values, such that acute toxicity is not

¹ A major component of CAS number 184378-08-3 is CAS number 68411-46-1

expected at or below their water solubility.

Mammalian Toxicology - Acute. There is a low concern for acute toxicity for all materials. Data are available for most members of the category indicating that the category has been well tested for acute mammalian effects.

Mammalian Toxicology - Mutagenicity. There is a low concern for mutagenicity either for aryl or alkyl substituted materials. Similarly, the data for a mixed aryl/alkyl substituted molecule also indicates a lack of mutagenicity. Data are available for several members of the category or close structural analogs, and these data can be bridged to the other members of the category.

Mammalian Toxicology – Repeated Dose Toxicity. Sufficient data are available to adequately represent the Substituted Diphenylamines for the purposes of the HPV Program.

Mammalian Toxicology - Reproductive and Developmental Toxicity. Sufficient data are available to adequately represent the Substituted Diphenylamines for the purposes of the HPV Program.

Conclusion. Based upon the data reviewed in the report, the physicochemical, environmental fate and toxicological properties of the Substituted Diphenylamine category members are similar and follow a regular pattern as a result of that structural similarity. Therefore, the EPA definition of a chemical category has been met.

Introduction

The category justification and the attached robust summaries in this submission are revisions of documents submitted in support of the Substituted Diphenylamines category on December 18, 2001 and August 5, 2003. In revising these documents, comments received from EPA (dated November 27, 2002) and Environmental Defense (dated May 15, 2003) have been considered. A provision for the use of structure activity relationships (SAR) to reduce testing needs is included under EPA's HPV Program. Specifically, categories may be formed based on structural similarity, through analogy, or through a combination of category and analogy for use with single chemicals. The benefits of using a category approach are numerous and include accelerated release of hazard information to the public; reduction in the number of animals used for testing; and an economic savings as a result of a reduced testing program.

The Substituted Diphenylamines materials that form this category based on structural similarity are:

Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)

Benzenamine, N-phenyl-, styrenated (68442-68-2)

Benzenamine, N-phenyl- (184378-08-3)²

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

Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)

² A major component of CAS number 184378-08-3 is CAS number 68411-46-1

Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)

The materials were further arranged in order of molecular weight, so that the smallest material is listed first, and materials listed subsequently have increasingly larger molecular weights. All of these materials are listed under the HPV Program.

Human exposure to Diphenylamine derivatives that are used as rubber and oil antidegradants at levels of 5% or less is minimal as a pesticide and as an edible residue. In addition, three of the chemicals in this category (68411-96-1, 68442-68-2 and 101-67-7) have FDA approvals.

The development of this category follows EPA guidance³.

Background Information: Manufacturing and Commercial Applications

Manufacturing

A common synthetic pathway in the production of Substituted Diphenylamines is via a process known as alkylation. The common starting material, Diphenylamine, (or Benzenamine, N-phenyl-) is reacted with an olefin containing the desired substituent group(s). The resulting reaction product is typically purified by distillation.

Commercial Applications

Substituted Diphenylamines materials are highly effective and active antioxidants in natural and many types of synthetic rubbers. They also impart heat-resistance and flex-fatigue resistance to rubber articles used in high-temperature and dynamic applications, such as under-the-hood automotive belts, gaskets and bushings. Because of their relatively non-staining and non-migratory nature, some Substituted Diphenylamines are used in the manufacture of light-colored rubber articles and adhesives that may contact food. Typical use percentage for a Substituted Diphenylamine in rubber compounding is 1-4 parts for every 100 parts of rubber. In heavy-duty functional fluids, Substituted Diphenylamines are powerful antioxidants that extend the useful life of transmission fluids, gear oils, lubricants and hydraulic fluids that must retain their properties in high-speed, high-temperature and/or high-load applications. Typical use percentage for a Substituted Diphenylamine as a functional fluid antioxidant is 1-4%.

Due to their powerful antioxidant properties, Substituted Diphenylamines, along with their common starting material, Diphenylamine, are regulated for use in several food-contact applications by the Food and Drug Administration as Indirect Food Additives under the following sections of 21 CFR:

175.105	Components of Adhesives	Diphenylamine, 101-67-7 and 68422-68-2
175.300	Resinous and Polymeric Coatings	Diphenylamine

³ US EPA, Office of Pollution Prevention and Toxics. Development of Chemical Categories, Chemical Right-to-Know Initiative. <http://www.epa.gov/opptintr/chemrtk/categuid.htm>

176.170	Components of Paper/Paperboard – Fatty Food	Diphenylamine
176.180	Components of Paper/Paperboard – Dry Food	Diphenylamine
177.1210	Closures with Sealing Gaskets	68411-46-1
177.2600	Rubber Articles	Diphenylamine, 101-67-7 68442-68-2
178.2010	Antioxidants/Stabilizers for Polymers	68411-46-1 68442-68-2
178.3570	Lubricants with Food Contact	68411-46-1

Shipping/Distribution

Substituted Diphenylamines materials are shipped extensively throughout the world from manufacturing plants in the USA, Eastern and Western Europe and Japan. Container types vary with physical form, quantity of material and destination. Boxes, bags of varying sizes, drums, tote tanks and tank cars can be used to transport Substituted Diphenylamines.

Worker/Consumer Exposure

The rubber and plastics additives industry has a long safety record and sophisticated users handle materials. Exposure of workers handling Substituted Diphenylamine materials is likely to be the highest in the areas of material packaging at the manufacturing site and during raw material weigh-up at the customer site. These materials are produced as dust-suppressed powders, flakes, and viscous liquids. Thus, during the above operations, there is some potential for inhalation exposure (nuisance dust is the primary route of worker exposure) and dermal contact.

Substituted Diphenylamines are industrial chemicals that are sold to industrial users only. Exposure to the consumer/general public would be slight to nil. Substituted Diphenylamines would be polymer-bound in a cured rubber product. Substituted Diphenylamines used in functional fluids represent a minor component of a complex mixture used in industrial applications.

Development of the Substituted Diphenylamines Category

EPA has described a stepwise process for developing categories. These steps include:

- Grouping a series of like chemicals, including the definition of criteria for the group.
- Gathering data on physicochemical properties, environmental fate and effects, and health effects for each member of the category.
- Evaluating the data for adequacy.
- Constructing a matrix of available and unavailable data.
- Determining whether there is a correlation among category members and data gathered.

Definition of the Substituted Diphenylamines Category

As defined by EPA under the HPV Program, a chemical category is “a group of chemicals whose physicochemical and toxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity.” The similarities should be based on a common functional group, common precursors or breakdown products (resulting in structurally similar chemicals) and an

incremental and constant change across the category. The goal of developing a chemical category is to use interpolation and/or extrapolation to assess chemicals rather than conducting additional and unnecessary testing.

The materials within the Substituted Diphenylamines category, for the purposes of the HPV Program, are defined as amines, which vary with the degree of alkyl (straight chain or branched) or phenyl groups, as illustrated in Figure 1. These materials differ by the type and extent of the substitution of the phenyl group, with either alkyl- or aryl substitution on the molecule, and in one instance, mixed alkyl/aryl substitution. Chemical structures for these materials are provided in Figure 2. The lack of water solubility, low vapor pressure, and inability to biodegrade are similar for the substituted diphenylamines (see Table 1). Furthermore, these materials are not flammable.

Matrix of SIDS Endpoints

In order to construct a matrix of SIDS endpoints for the members of the substituted diphenylamines category, the data on physicochemical properties, environmental fate and effects, and health effects for each member of the category must be collected and evaluated for adequacy. The results of these activities are presented in the tables and text below, providing a matrix of available data.

Correlation within the Substituted Diphenylamines Category

The matrix data patterns for physicochemical properties; environmental fate, ecotoxicity; and health effects have been evaluated for the members of the Substituted Diphenylamine category. A description of the results of this evaluation follows.

Correlation of Physicochemical Properties

The physicochemical properties of the members of the Substituted Diphenylamine category are presented in Table 2. These materials may exist as liquids or solids at room temperature, such that melting point or boiling point data may not be relevant for varying members of the category. The similarities in the other physicochemical properties of these materials, which are described below, are explained by similarities in their chemical structure, and provide justification of this group of chemicals as a category within the HPV Challenge Program.

The members of this category have a wide range of melting points and boiling points (varying based on the physical state as a liquid or solid). All the members of this category have very low vapor pressures, as indicated in Table 2. Data for the members of this category clearly indicate a lack of water solubility or negligible water solubility. Partition coefficient data fall into two ranges; from ~4 to 6 and from ~10 to 12.

For the purposes of the HPV Program, bridging to other members of the category addressed outstanding physicochemical properties data requirements, as illustrated below.

- The vapor pressure for Benzenamine, 4-octyl-N-(4-octylphenyl) (101-67-7) was bridged to:
 - Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3) and
 - Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]- (10081-67-1)

-
- The water solubility for Benzenamine, 4-octyl-N-(4-octylphenyl) (101-67-7) was bridged to Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)
 - The partition coefficient for Benzenamine, 4-octyl-N-(4-octylphenyl) (101-67-7) was bridged to:
 - Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3) and
 - Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]- (10081-67-1)

Correlation of Environmental Fate

The members of this category are found to be not readily biodegradable, have rapid photodegradation half-lives, and modeling shows a primary partitioning to soil and sediment fractions (vs. water) (Table 3). Hydrolysis data are not available for these materials, as discussed below.

The HPV Challenge Program requires that hydrolysis, photodegradation, biodegradation and environmental transport information be presented for each material or bridged to each member of a category. Adequate biodegradation data exist for the several of the materials in this category; bridging will be used to address the remaining biodegradation data requirements as illustrated below. The results presented indicate that these materials are poorly biodegradable. Hydrolysis testing of the members of this category is not appropriate since they are not water-soluble. Photodegradation studies presented for several members of this category are adequate; bridging will be used to fill the remaining photodegradation data requirements as illustrated below. Finally, fugacity modeling has been conducted on several of the members of this category, with consistent results showing partitioning to soil and sediment; with the exception noted above for diphenylamine. This is consistent with the lack of water solubility and low vapor pressure of these materials. For the purposes of the HPV Program, bridging to other members of the category will address outstanding environmental fate data requirements, as illustrated below.

- The photodegradation information from Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1) and Benzenamine, N-phenyl- (184378-08-3) was bridged to:
 - Benzenamine, N-phenyl-, styrenated (68442-68-2) and
 - Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1).
- The photodegradation information from Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5) was bridged to:
 - Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7) and,
 - Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3).
- The biodegradation data from Benzenamine, N-phenyl-, styrenated (68442-68-2) and Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3) was bridged to:
 - Benzenamine, N-phenyl- (184378-08-3), and
 - Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7) and
 - Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1).
- The biodegradation data from Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3) was bridged to:
 - Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5) and

-
- Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9).
 - Environmental Transport modeling was bridged from Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1) to:
 - Benzenamine, N-phenyl-, styrenated (68442-68-2) and
 - Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1).
 - Environmental Transport modeling was bridged from Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5) to:
 - Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7) and
 - Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3).

Correlation of Ecotoxicity

The HPV Challenge Program requires that an acute aquatic ecotoxicity test in fish, invertebrates, and algae be performed or bridged to each member of a category. Existing data (Table 2) indicate that all members of the Substituted Diphenylamine category have low water solubility. The low water solubility suggests that the acute aquatic toxicity of these materials should be low due to limited bioavailability to aquatic organisms. These materials have high estimated log Kow values, such that acute toxicity is not expected at or below their water solubility. Sufficient data are available to meet HPV Program requirements for the toxicity of the Substituted Diphenylamines to aquatic organisms (Table 4). As the molecular weight of the category members increases, there is a clear reduction in the acute aquatic toxicity of these materials. For the purposes of the HPV Program, bridging from this data was used to address the data information requirements for the remainder of this category as illustrated below.

- The data for Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7), Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1), Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3), and Benzenamine, N-phenyl-, styrenated (68442-68-2) was bridged to the remaining members of this category.

Correlation of Health Effects

Acute Mammalian Toxicity

Acute oral and dermal toxicity data for the category are summarized in Table 5. Of the Substituted Diphenylamines tested, all show a slight to very low order of toxicity following oral administration, with LD₅₀ values ranging from >500 to > 34,000 mg/kg. Overall, the acute dermal LD₅₀ for these materials was greater than the 2000 mg/kg limit dose indicating a very low order of toxicity.

Numerous adequate acute toxicity studies have been conducted for the Substituted Diphenylamine category using two routes of exposure (oral and dermal); and the toxicity of four of the nine members of the category has been evaluated. The data demonstrate a slight to very low order of acute toxicity. The similarity in the order of toxicity for these materials is consistent with their similar chemical structure and physicochemical properties and supports the scientific justification of these materials as a category within the HPV Challenge Program.

The HPV Challenge Program requires that either an acute test be performed or bridged to each member of a category. Adequate acute oral toxicity tests exist for four of the Substituted Diphenylamines; for the purposes of the HPV Program, bridging was used to fill the remaining data requirements as follows.

- Acute oral toxicity data from Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1) will be bridged to Benzenamine, N-phenyl- (184378-08-3)
- Acute oral toxicity data from Benzenamine, N-phenyl-, styrenated (68442-68-2) was bridged to Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1).
- Acute oral toxicity data from Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7) was bridged to Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3).
- Acute oral toxicity data from Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5) was bridged to Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9).

By bridging existing data to the materials for which data were not identified, the acute toxicity of the category has met requirements of the HPV Program with respect to all acute toxicity endpoints.

Mutagenicity

A summary of the mutagenicity information for the Substituted Diphenylamines category is presented in Table 6. The weight of evidence for the members of this category indicates these materials are not mutagenic.

Adequate bacterial mutagenicity tests exist for five of the Substituted Diphenylamines category; bridging will be used to address the remaining data requirements for the purposes of the HPV Program. Adequate *in vitro* chromosome aberration tests or *in vivo* micronucleus tests exist for two of the materials in the Substituted Diphenylamines category; bridging will be used to address the remaining data requirements. Bacterial and mammalian mutagenicity studies are available for aryl (for example, CAS No. 68442-68-2) and alkyl (for example, CAS No. 101-67-7) substituted diphenylamines. Furthermore, a bacterial mutagenicity study is also available for a mixed aryl/alkyl substituted phenylenediamine (CAS No. 68921-45-9). Each of these studies indicates a clear lack of mutagenicity of these materials, whether the substitution is alkyl (straight chain or branched), aryl or mixed alkyl/aryl.

Bacterial Gene Mutation Assay

Overall weight of evidence for the category indicates a negative evaluation for bacterial mutagenicity.

In vitro or In vivo Chromosomal Aberration Assays

Two (one alkyl and one aryl substituted) of the Substituted Diphenylamine materials have been adequately tested in an *in vitro* or *in vivo* chromosomal aberration assay to satisfy HPV requirements. These test materials were negative for clastogenicity.

The Substituted Diphenylamines category has been tested for mutagenicity in tests for gene mutations and chromosomal aberrations. The assays included point mutations in bacterial cells, *in vitro* chromosomal aberrations in mammalian cells, and *in vivo* chromosomal aberrations. The data consistently demonstrate no evidence of genotoxicity for this category of materials. This suggests that

all members of the category lack genotoxicity due to their similarity in chemical structures and physicochemical properties. The similarity of results for genotoxicity supports treatment of these materials as a chemical category within the HPV Challenge Program.

The HPV Challenge Program requires that a gene mutation and a chromosomal aberration test be performed or bridged to each member of a category. For the purposes of the HPV Program, bridging was used to address the remaining data requirements.

- Bacterial and in vivo mammalian mutagenicity data was bridged from Benzenamine, N-phenyl-, styrenated (68442-68-2) to Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)
- Bacterial and in vitro mammalian mutagenicity data was bridged from Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7) to:
 - Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3) and
 - Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1), and
- In vitro mammalian mutagenicity data was bridged from Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7) to:
 - Benzenamine, N-phenyl- (184378-08-3), and
 - Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5).
- In vivo and in vitro mammalian mutagenicity data was bridged from Benzenamine, N-phenyl-, styrenated (68442-68-2) and Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7) to Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9).

By bridging these data, the category has met the requirements of the HPV Challenge Program.

Repeat Dose Toxicity

A summary of the repeat dose toxicity data for the Substituted Diphenylamines category is presented in Table 7.

Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9) was tested in a 64 week rat dietary study; a LOEL of 2500 ppm was identified. A 28-day repeat dose toxicity study with screening developmental and reproductive endpoints (OECD 422) was conducted for Benzenamine, N-phenyl-, styrenated (68442-68-2), which is the smallest aryl substituted compound and Benzenamine, N-phenyl- (184378-08-3), which is the smallest alkyl substituted compound in the category (as mentioned previously, a major component of CAS number 184378-08-3 is CAS number 68411-46-1). The NOAEL for Benzenamine, N-phenyl-, styrenated (68442-68-2) was 600 mg/kg bw/d; the NOAEL for Benzenamine, N-phenyl- (184378-08-3) was 5 mg/kg bw/d.

Reproductive and Developmental Toxicity

A summary of the reproductive/developmental toxicity data for the Substituted Diphenylamines category is presented in Table 7.

Standard reproductive and developmental toxicity data are provided for Benzenamine, N-phenyl-, styrenated (68442-68-2) and Benzenamine, N-phenyl- (184378-08-3), through the conduct of OECD TG 422 studies (Table 7). The NOAEL for reproductive effects, maternal toxicity and developmental effects was 250 mg/kg bw/d for Benzenamine, N-phenyl-, styrenated (68442-68-2). The NOAEL for reproductive effects and maternal toxicity was 5 mg/kg bw/d; the NOAEL for developmental effects was 25 mg/kg bw/d for Benzenamine, N-phenyl- (184378-08-3).

Test Plan

Table 8 provides the completed category test plan for the Substituted Diphenylamines.

FIGURES

Figure 1. Substituted Diphenylamine Structural Definition

Mononitrogen (N) containing with various degrees of phenyl or alkyl substitution:

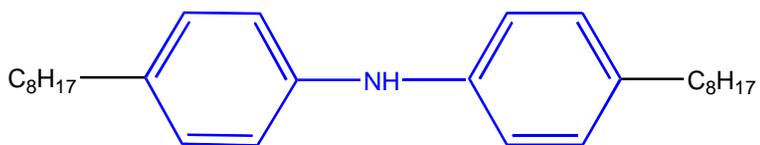


Where:

Ph = phenyl;

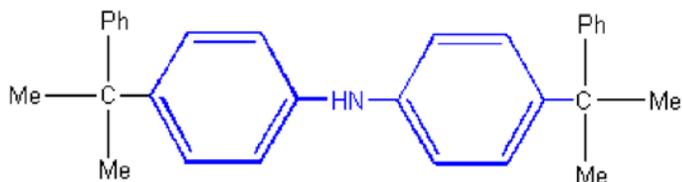
R,R' =butyl derivatives, octyl-derivatives, nonyl-derivatives, styrenyl-derivatives

Figure 2 Substituted Diphenylamine Chemical Structures



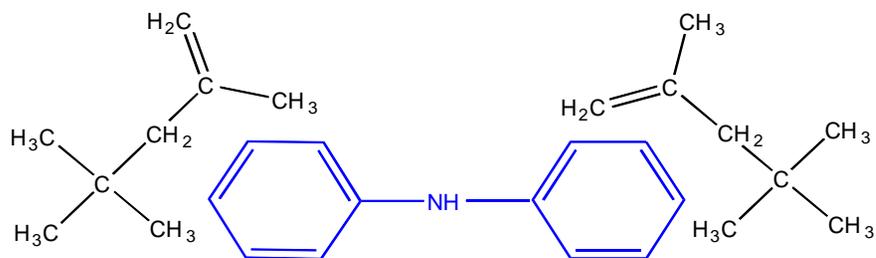
101-67-7

Benzenamine, 4-Octyl-N-(4-octylphenyl)-



10081-67-1

Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]-

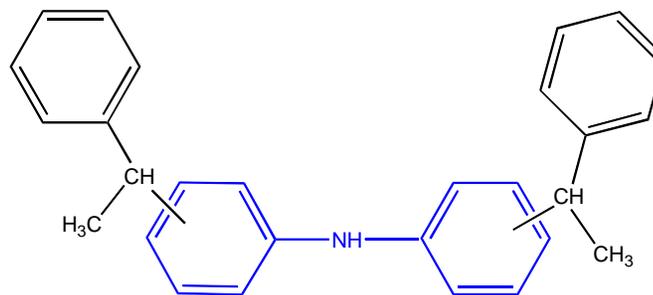


68411-46-1

[Ring attachment at #2 carbon]

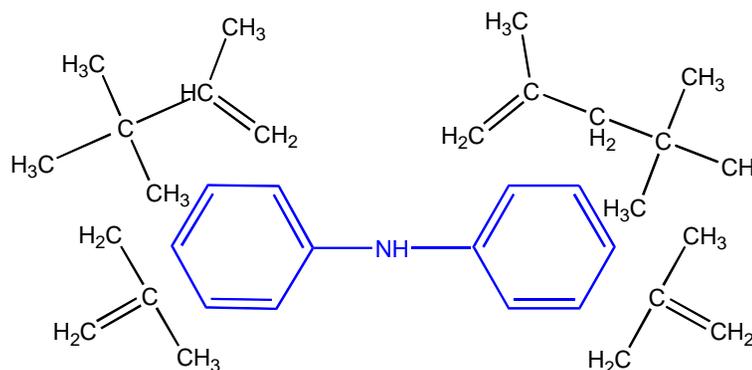
Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene

Figure 2 Substituted Diphenylamine Chemical Structures (continued)



68442-68-2

Benzenamine, N-phenyl-, styrenated

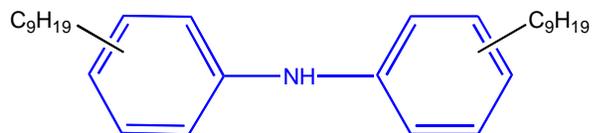


184378-08-3

[Ring attachment at #2 carbon]

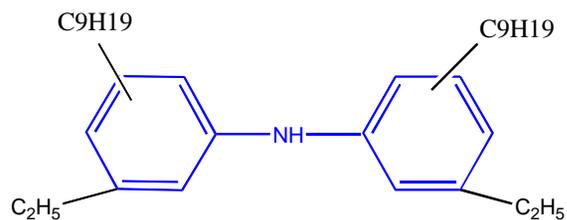
Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene and isobutylene

Figure 2 Substituted Diphenylamine Chemical Structures (continued)



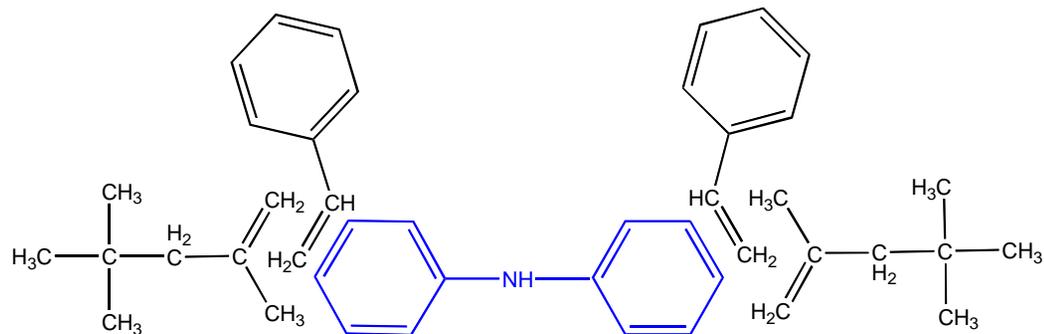
36878-20-3

Benzenamine, ar-nonyl-N-(nonylphenyl)-
Mixed Dinonyldiphenylamines



68608-77-5

[alkylation reaction of diethyldiphenylamine with propylene trimer]
Benzenamine, 2-Ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives



68921-45-9

[Ring attachment at #2 carbon]

Benzenamine, N-Phenyl, reaction products with Styrene and 2,4,4-Trimethylpentene

TABLES

Table 1. Justification of the Substituted Diphenylamines Category using Flash Point, Vapor Pressure, Water Solubility and Biodegradation

Name (CAS No.)/ Molecular weight	Substitution	Flash Point (°C)	Vapor Pressure	Water Solubility	Biodegradability
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)/ 298-350	Alkyl	Not determined	2E-5 mm Hg @ 25 °C	Very low	Not determined
Benzenamine, N-phenyl-, styrenated (68442-68-2)/ 320	Aryl	270	<100 hPa @50°C	Very low	Not readily biodegradable
Benzenamine, N-phenyl- (184378-08-3)/225-393 ⁴	Alkyl	>180	2E-5 mm Hg @ 25 °C	Very low	Not determined
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)/ 394	Alkyl (branched)	Not determined	<0.13332 hPa	Very low	Not readily biodegradable
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1) /406	Aryl	276.7	Not determined	Insoluble	Not determined
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3) / 422	Alkyl (branched)	Not determined	Not determined	Not determined	Not determined
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)/ 225-479	Alkyl	213	2.35E-8 to 9.18E-12 hPa @25C EPIWin	Insoluble	Not determined
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)/ 225-633	Mixed Alky/Aryl	180	9.99E-7 to 1.9E-15 hPa EPIWin	Negligible	Not determined

⁴A major component of CAS number 184378-08-3 is CAS number 68411-46-1

Table 2. Matrix of Available and Adequate Data on Substituted Diphenylamines Category Members Physicochemical Properties

Name (CAS No.)	Melting Point (°C)	Vapor Pressure (mm Hg @ 20°C)	Boiling Point (°C)	Partition Coefficient	Water Solubility (mg/L)
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	44-107	2E-5 @25 °C	~370 EPIWin	>6	<0.01% @ 20 °C
Benzenamine, N-phenyl-, styrenated (68442-68-2)	~6	<100 hPa @50°C	>300 @1013 hPa	4.64	0.41 @ 20C
Components of Benzenamine, N-phenyl-, styrenated (68442-68-2)	-	-	-	-	20.6 µg/L for p-SDPA < 58.8 µg/L (< LOQ) for p,p'-diSDPA < 27.6 µg/L (< LOQ) for o,p,p'-triSDPA
Benzenamine, N-phenyl- (184378-08-3) ⁵	44-107	2E-5 @25 °C	168	>6	<0.01%
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	87-95	<0.13332 hPa	200	11.26	<0.1 g/100 ml @21C
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)	98.5	Not determined	Not applicable; substance is a solid	Not determined	Insoluble
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	<0C	Not determined	258	Not determined	Not determined
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	<0C	2.35E-8 to 9.18E-12 hPa @25C	221	9.84	2.35E-5 to 5.85E-10 @25C EPIWin
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-	<0C	9.99E-7 to 1.9E-15 hPa	>198 175	5.2	0.3889 to 1.869E-11 @

⁵ A major component of CAS number 184378-08-3 is CAS number 68411-46-1

trimethylpentene (68921-45-9)		EPIWin			25C EPIWin
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Table 3. Matrix of Available and Adequate Data on Substituted Diphenylamines Category Members Environmental Fate

Name (CAS No.)	Hydrolysis	Photo-degradation (t1/2 in hours)	Biodegradation	Environmental Transport
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	Not determined	0.053 hours (EPIWin)	Not determined	Primarily to soil and sediment
Benzenamine, N-phenyl-, styrenated (68442-68-2)	Not determined	Not determined	9% after 28 days	Not determined
Benzenamine, N-phenyl- (184378-08-3) ⁶	Not determined	0.053 days (EPIWin)	Not determined	Primarily to soil and sediment
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	Not determined	0.049 days EPIWin	0.78% EPIWin	Primarily to soil and sediment
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)	Not determined	Not determined	Not determined	Not determined
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	Not determined	Not determined	8% after 28 days	Not determined
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	Not determined	0.05 to 0.048 days (EPIWin)	Not determined	Primarily to soil and sediment
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	Not determined	0.051 to 0.053 days (EPIWin)	Not determined	Primarily to soil and sediment

⁶ A major component of CAS number 184378-08-3 is CAS number 68411-46-1

Table 4. Matrix of Available and Adequate Data on Substituted Diphenylamines Category Members Ecotoxicity

Name (CAS No.)	Acute Fish 96-hour LC50 (mg/l)	Acute Invertebrate 48-hour EC50 (mg/l)	Algal growth inhibition EC50 (mg/l)
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	Not determined	Not determined	Not determined
Benzenamine, N-phenyl-, styrenated (68442-68-2)	920	Not determined	Not determined
Benzenamine, N-phenyl- (184378-08-3) ⁷	Not determined	Not determined	Not determined
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	>1000	7.7	>100 (growth rate)
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)	Not determined	Not determined	Not determined
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	>10,000	733	600 (growth rate)
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	Not determined	Not determined	Not determined
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	Not determined	2.3 (96 hrs) mysid shrimp	Not determined

⁷ A major component of CAS number 184378-08-3 is CAS number 68411-46-1

**Table 5. Matrix of Available and Adequate Data on Substituted Diphenylamines Category Members
Acute Toxicity**

Name (CAS No.)	Acute Oral (mg/kg)	Acute Dermal (mg/kg)
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	Not determined	Not determined
Benzenamine, N-phenyl-, styrenated (68442-68-2)	>20,000	>10,000
Benzenamine, N-phenyl- (184378-08-3) ⁸	>2500	Not determined
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	>7940	>7940
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)	Not determined	Not determined
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	Not determined	Not determined
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	>34,600	>3000
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	Not determined	Not determined

⁸ A major component of CAS number 184378-08-3 is CAS number 68411-46-1

Table 6. Matrix of Available and Adequate Data on Substituted Diphenylamines Category Members Genotoxicity

Name (CAS No.)	Genotoxicity (<i>in vitro</i> bacterial)	Genotoxicity (<i>in vitro</i> mammalian)	Genotoxicity (<i>in vivo</i>)
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	Not determined	Not determined	Not determined
Benzenamine, N-phenyl-, styrenated (68442-68-2)	Negative	Not determined	Negative
Benzenamine, N-phenyl- (184378-08-3) ⁹	Negative	Not determined	Not determined
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	Negative	Negative	Ambiguous
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)	Not determined	Not determined	Not determined
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	Not determined	Not determined	Not determined
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	Negative	Not determined	Not determined
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	Negative	Not determined	Not determined

⁹A major component of CAS number 184378-08-3 is CAS number 68411-46-1

**Table 7. Matrix of Available and Adequate Data on Substituted Diphenylamines Category Members
Repeat dose, Reproductive and Developmental Effects**

Name (CAS No.)	Repeat Dose	Reproductive	Developmental
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	Not determined	Not determined	Not determined
Benzenamine, N-phenyl-, styrenated (68442-68-2)	OECD 422; NOAEL = 600 mg/kg bw/d	OECD 422; NOAEL = 250 mg/kg bw/d	OECD 422; NOAEL = 250 mg/kg bw/d
Benzenamine, N-phenyl- (184378-08-3)	OECD 422; NOAEL = 5 mg/kg bw/d	OECD 422; NOAEL = 5 mg/kg bw/d	OECD 422; NOAEL = 5 mg/kg bw/d (maternal toxicity); =25 (developmental effects)
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	Not determined	Not determined	Chicken Embryos, NOEL 1 uMol/egg
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)	Not determined	Not determined	Not determined
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	Not determined	Not determined	Not determined
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	Not determined	Not determined	Not determined
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	64 week rat dietary study LOEL = 2500 ppm	Not determined	Not determined

Table 8
Substituted Diphenylamines Category
Final Submittal

CAS Nos. 68411-46-1, 68442-68-2, 184378-08-3, 101-67-7, 10081-67-7
36878-20-3, 68608-77-5 and 68921-45-9
Rubber and Plastic Additives Panel, American Chemistry Council
Revised October 2006

Legend	
Symbol	Description
R	Endpoint requirement fulfilled using category approach, SAR
Test	Endpoint requirements to be fulfilled with testing
Calc	Endpoint requirement fulfilled based on calculated data
A	Endpoint requirement fulfilled with adequate existing data
NA	Not applicable due to physical/chemical properties

CHEMICAL	Physical-Chemical				
	Melting Point	Boiling Point	Vapor Pressure	Partition Coefficient	Water Solubility
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	A	A	A	A	A
Benzenamine, N-phenyl-, styrenated (68442-68-2)	A	A	A	A	A
Benzenamine, N-phenyl- (184378-08-3) ¹⁰	A	A	A	A	A
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	A	A	A	A	A
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]- (10081-67-1)	A	NA (substance is a solid)	R	R	R
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	A	A	R	R	R
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	A	A	A	A	A
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	A	A	A	A	A

¹⁰ A major component of CAS number 184378-08-3 is CAS number 68411-46-1

Table 8 (continued)

CHEMICAL	Environmental Fate			
	Photodegradation	Hydrolysis	Environmental Transport	Biodegradation
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	A(Calc)	NA	A(Calc)	R
Benzenamine, N-phenyl-, styrenated (68442-68-2)	R	NA	R	A
Benzenamine, N-phenyl- (184378-08-3)	A(Calc)	NA	A(Calc)	R
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	R	NA	A	A
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]- (10081-67-1)	R	R	R	R
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	R	NA	R	A
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	A(Calc)	NA	A(Calc)	R
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	A(Calc)	NA	A(Calc)	R

Table 8 (continued)

CHEMICAL	Ecotoxicity		
	Acute Toxicity to Fish	Acute Toxicity to Algae	Acute Toxicity to Aquatic Invertebrates (e.g., Daphnia)
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	R	R	R
Benzenamine, N-phenyl-, styrenated (68442-68-2)	A	R	R
Benzenamine, N-phenyl- (184378-08-3)	R	R	R
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	A	A	A
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)	R	R	R
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	A	A	A
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	R	R	R
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	R	R	R

Table 8 (continued)

CHEMICAL	Toxicity						
	Acute Toxicity	Genetic Toxicity <i>In Vitro</i> (bacterial)	Genetic Toxicity <i>In Vitro</i> (mammalian)	Genetic Toxicity <i>In Vivo</i>	Repeat Dose Toxicity	Reproductive Toxicity	Developmental Toxicity
Benzenamine, N-Phenyl-, reaction products with 2,4,4-trimethylpentene (68411-46-1)	R	R	R	R	R	R	R
Benzenamine, N-phenyl-, styrenated (68442-68-2)	A	A	R	A	A	A	A
Benzenamine, N-phenyl- (184378-08-3)	A	A	R	R	A	A	A
Benzenamine, 4-Octyl-N-(4-octylphenyl) (101-67-7)	A	A	A	R	R	R	R
Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl) phenyl]- (10081-67-1)	R	R	R	R	R	R	R
Benzenamine, ar-nonyl-N-nonylphenyl (36878-20-3)	R	R	R	R	R	R	R
Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives (68608-77-5)	A	A	R	R	R	R	R
Benzenamine, N-Phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (68921-45-9)	R	A	R	R	A	R	R