

201-15003B

I U C L I D

Data Set

04 JAN - 6 PM 2:32

RECEIVED
DUPT. CRIC

Existing Chemical : ID: 123-18-2
Memo : Isobutyl Heptyl Ketone (IBHK)
CAS No. : 123-18-2
EINECS Name : 2,6,8-Trimethylnonan-4-one
EC No. : 204-607-3
TSCA Name : 4-Nonanone, 2,6,8-trimethyl-
Molecular Formula : C₁₂H₂₄O

Producer related part

Company : The Dow Chemical Company
Creation date : 12.09.2003

Substance related part

Company : The Dow Chemical Company
Creation date : 12.09.2003

Status :
Memo :

Printing date : 18.12.2003
Revision date :
Date of last update : 18.12.2003

Number of pages : 20

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. General Information

Id 123-18-2
Date 18.12.2003

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

IUPAC Name :
Smiles Code : O=C(CC(CC(C)C)C)CC(C)C
Molecular formula : C₁₂H₂₄O₁
Molecular weight : 184.32
Petrol class :

05.12.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : liquid
Purity : -
Colour : transparent colorless
Odour : obnoxious

Remark : Purity/Composition:
>=95 and <=100% 2,6,8-Trimethyl-4-nonanone
<= 4% 4-Nonanol, 2,6,8-trimethyl-

11.12.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2,6,8-Trimethyl-4-nonanone

15.12.2003

2,6,8-Trimethylnonan-4-one

15.12.2003

4-Nonanone, 2,6,8-Trimethyl-

15.12.2003

ECOSOFT Solvent IK

18.12.2003

Isobutyl heptyl ketone (IBHK)

15.12.2003

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. General Information

Id 123-18-2
Date 18.12.2003

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 : = -75.2 - °C

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.12.2003 (2)

2.2 BOILING POINT

Value : = 218.3 - °C at 1013 hPa

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.12.2003 (2)

2.3 DENSITY

Type : density

Value : = .818 - g/cm³ at 20 °C

09.10.2003 (2)

2.3.1 GRANULOMETRY**2.4 VAPOUR PRESSURE**

Value : = .07413 - hPa at 20 °C

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.12.2003 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water

Log pow : = 3.96 - at °C

pH value : -

Method : other (calculated): EPIWIN (v 3.11) KOWWIN Submodel (v 1.67)

Year : 2003

GLP :

Test substance :

Remark : The EPIWIN model was run using the following measured physical chemical properties:
Water solubility (mg/L) = 22;
Vapor pressure (mm Hg) = 0.05574;
Boiling point (deg C) = 218.25; and
Melting point (deg C) = -75.15.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

2. Physico-Chemical Data

Id 123-18-2
Date 18.12.2003

09.12.2003

(4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 22 - mg/l at 20 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: broadly covered by ASTM method E 1148
Year : 2000
GLP : yes
Test substance : other TS

Remark : The liquid-liquid equilibrium measurements were performed in a 0.5 liter glass vessel in a constant-temperature bath. Water and IBHK were added to this vessel through 1/16" lines. The mixture was then stirred vigorously by a magnetic stirrer at the desired bath temperature. Stirring produced very fine droplets of each phase entrained in the other phase, which slowly separated after the liquid was still. After the liquid phases had separated, at least three 10-20 gram samples were withdrawn from both the organic and aqueous liquid phase into weighed glass bottles. A weighed amount of a mixture of toluene and ethylbenzene was added to each vial, and the IBHK was extracted into the toluene-rich phase by vigorously shaking the vial. Ethylbenzene served as the internal standard. An aliquot of the toluene-rich phase was then analyzed by gas chromatography. The concentration of water was found by difference. The hydrocarbon-rich samples were analyzed for water by Karl Fisher titration. 2-Methoxyethanol was added, if necessary, to the sample to prevent a second liquid phase from forming.

The gas chromatographic analyses were performed by an HP5890A gas chromatograph equipped with a DB-1 capillary column. The column was 30 meters long with an internal diameter of 0.32 millimeters and a film thickness of 3 micrometers. Response factors were determined by analyzing gravimetrically prepared standards before each set of samples.

Result : In all samples of the flask shaking test there was excellent separation of the phases. Results were repeated in triplicate. Compositions between 1.0 wt% (10,000 ppm) and 0.1 wt% (1000 ppm) are estimated to be reliable to $\pm 5\%$ of the reported value. The uncertainty increases to $\pm 20\%$ of the reported value as the measured compositions decrease to lower ppm concentrations. The measured value for IBHK was 0.0022 wt% (22 ppm).

Test substance : ECOSOFT Solvent IK: purity > 96 wt. %
This purity is actually measured for isobutyl heptyl ketone + isomers + trimethyl nonanol (CAS RN 123-17-1)

Reliability : (1) valid without restriction
Comparable to guideline study.

Flag : Critical study for SIDS endpoint

09.12.2003

(6)

2.6.2 SURFACE TENSION

2. Physico-Chemical Data

Id 123-18-2
Date 18.12.2003

2.7 FLASH POINT

Value : = 82.9 °C
Type :

09.12.2003

(2)

2.8 AUTO FLAMMABILITY

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

Type : other: EPIWIN (v 3.11) AOPWIN Submodel (v 1.91)
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
DIRECT PHOTOLYSIS
Half-life t1/2 : = 5.5 - hour(s)
Degradation : - % after
Quantum yield :
Deg. product :
Method : other (calculated): EPIWIN (v 3.11) AOPWIN Submodel (v 1.91)
Year : 2003
GLP :
Test substance :

Remark : Overall OH rate constant = 23.2 E-12 cm³/molecule/sec
The EPIWIN model was run using the following measured physical
chemical properties:
Water solubility (mg/L) = 22;
Vapor pressure (mm Hg) = 0.05574;
Boiling point (deg C) = 218.25; and
Melting point (deg C) = -75.15.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
11.12.2003 (3)

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

Media : other: air (emissions to compartment = 1000 kg/hr)
Method : Calculation according Mackay, Level III
Year : 2003

Method : Equilibrium Concentration Model (EQC) Level III.

The EPIWIN model was run using the following measured physical
chemical properties:
Water solubility (mg/L) = 22;
Vapor pressure (mm Hg) = 0.05574;
Boiling point (deg C) = 218.25; and

3. Environmental Fate and Pathways

Id 123-18-2
Date 18.12.2003

Remark : Melting point (deg C) = -75.15.
: Level III Fugacity Model (Full-Output):
=====

Chem Name : 4-Nonanone, 2,6,8-trimethyl-
Molecular Wt: 184.32
Henry's LC : 0.000614 atm-m³/mole (calc VP/Wsol)
Vapor Press : 0.0557 mm Hg (user-entered)
Log Kow : 3.96 (Kowwin program)
Soil Koc : 3.74e+003 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	95.8	11	1000
Water	2.89	360	0
Soil	1.09	360	0
Sediment	0.173	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.82e-011	861	137	86.1	13.7
Water	6.86e-012	0.797	0.414	0.0797	0.0414
Soil	3.22e-013	0.301	0	0.0301	0
Sediment	2.28e-012	0.0119	0.000496	0.00119	4.96e-005

Persistence Time: 14.3 hr
Reaction Time: 16.6 hr
Advection Time: 104 hr
Percent Reacted: 86.2
Percent Adverted: 13.8

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 11.05
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.769 (weeks)

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

Result : Concentration (%):
Air - 96
Water - 3
Soil - 1
Sediment - < 1

Reliability Flag : (2) valid with restrictions
: Critical study for SIDS endpoint
09.12.2003 (5)

Media Method Year : other: water (emissions to compartment = 1000 kg/hr)
: Calculation according Mackay, Level III
: 2003

Method : Equilibrium Concentration Model (EQC) Level III.

The EPIWIN model was run using the following measured physical chemical properties:
Water solubility (mg/L) = 22;
Vapor pressure (mm Hg) = 0.05574;
Boiling point (deg C) = 218.25; and
Melting point (deg C) = -75.15.

3. Environmental Fate and Pathways

Id 123-18-2
Date 18.12.2003

Remark : Level III Fugacity Model (Full-Output):

=====
Chem Name : 4-Nonanone, 2,6,8-trimethyl -
Molecular Wt: 184.32
Henry's LC : 0.000614 atm-m³/mole (calc VP/Wsol)
Vapor Press : 0.0557 mm Hg (user-entered)
Log Kow : 3.96 (Kowwin program)
Soil Koc : 3.74e+003 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.25	11	0
Water	92.2	360	1000
Soil	0.0256	360	0
Sediment	5.52	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	6.84e-012	324	51.6	32.4	5.16
Water	3.5e-009	407	211	40.7	21.1
Soil	1.21e-013	0.113	0	0.0113	0
Sediment	1.16e-009	6.09	0.253	0.609	0.0253

Persistence Time: 229 hr
Reaction Time: 311 hr
Advection Time: 871 hr
Percent Reacted: 73.7
Percent Advected: 26.3

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 11.05
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.769 (weeks)

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

Result : Concentration (%):

Air - 2
Water - 92
Soil - <0.1
Sediment - 6

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.12.2003

(5)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3. Environmental Fate and Pathways

Id 123-18-2
Date 18.12.2003

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

Type : LD50
Value : = 8470 - mg/kg bw
Species : rat
Strain : no data
Sex : male
Number of animals : 40
Vehicle : other: Tergitol 7
Doses : 6300, 7950, 10000 and 12600 mg/kg
Method : other: see remark
Year : 1948
GLP : no
Test substance : other TS

Remark : A 20% dispersion of the test substance in 1% Tergitol 7 was administered by gavage to 10 male albino rats per group. Doses were 6300, 7950, 10000 and 12600 mg/kg body weight. Animals were observed for 14 days following dosing. Body weights were obtained on the day of dosing and on day 14.

Result : LD50 = 8470 mg/kg (95% confidence limits = 7180 to 9990 mg/kg)

High doses resulted in prostration and narcosis, with lung hemorrhages, congested livers, pale kidneys and opacity of the intestine notable on autopsy. Death was delayed for 72 hours or more in most cases. All surviving animals gained weight 14 days following dosing. The number of deaths are indicated in the following table:

Dose (mg/kg)	Number dead/number dosed
6300	3/10
7950	4/10
10000	6/10
12600	10/10

Test substance : Trimethyl nonanone
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
 15.12.2003

(1)

5.1.2 ACUTE INHALATION TOXICITY

Type : other: saturated vapor
Value : -
Species : rat
Strain : no data
Sex : no data
Number of animals : 6
Vehicle :
Doses : substantially saturated vapor
Exposure time : 8 hour(s)
Method :
Year : 1948
GLP : no
Test substance : other TS

5. Toxicity

Id 123-18-2

Date 18.12.2003

Method	: Six rats were exposed to the test substance as a saturated vapor generated at room temperature for 8 hours.	
Result	: Two of the six rats died in 8 hours. The cause of death was considered to be direct damage to the lung, as revealed by marked congestion.	
Test condition 15.12.2003	: Trimethyl nonanone	(1)
Type	: other	
Value	: -	
Species	: rat	
Strain	: no data	
Sex	: no data	
Number of animals	: 6	
Vehicle	:	
Doses	: cooled mist	
Exposure time	: 1 hour(s)	
Method	: other: see remark	
Year	: 1948	
GLP	: no	
Test substance	: other TS	
Remark	: Six rats were exposed to the test substance as a cooled mist prepared by heating the aerated test substance to 170 degrees C.	
Result	: Exposure to a cooled mist was lethal to all of 6 rats in one hour and 0 of 6 rats in 30 minutes. The cause of death was considered to be direct damage to the lung, as revealed by marked congestion.	
Test condition 15.12.2003	: Trimethyl nonanone	(1)

5.1.3 ACUTE DERMAL TOXICITY

Type	: LD50	
Value	: = 9030 - mg/kg bw	
Species	: rabbit	
Strain	: no data	
Sex	: male	
Number of animals	: 40	
Vehicle	: other: none	
Doses	: 7950, 10000, 12600 and 15800 ml/kg	
Method	: other: see remark	
Year	: 1948	
GLP	: no	
Test substance	: other TS	
Remark	: The undiluted test substance was applied as a single dose to 4 groups of 10 male albino rabbits each at the following dose levels: 7950, 10000, 12600 and 15800 ml/kg, which correlates to doses of 6500, 8180, 10300 and 12900 mg/kg, respectively (density = 0.818 g/cm ³). The test material was applied, undiluted at the appropriate dose, under an impervious sheeting. The animals remained exposed to the test substance for 24 hours. Rabbits were observed for 14 days and body weights were obtained on the day of application and on day 14.	
Result	: LD50 = 9030 mg/kg (95% confidence limits = 7710 to 10590 mg/kg) Erythema and occasionally necrosis of the skin resulted from the dose. The animals were sensitive to handling for a period of one week after the application. All but 2 animals (one each in the 10300 and 6500 mg/kg dose groups) lost weight during the 14 day post-application period. The weight losses may have been attributed in part to persistent diarrhea. The number of deaths are indicated in the following table:	

	Dose (ml/kg)	Number dead/number dosed
	7950	2/10
	10000	4/10
	12600	5/10
	15800	9/10
Test substance	:	Trimethyl nonanone
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint
15.12.2003		

(1)

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

- (1) Carpenter, C.P. 1948. The Acute Toxicity of Trimethyl Nonanone. Unpublished Report Number 11-90. Mellon Institute of Industrial Research, University of Pittsburgh, PA, USA.
- (2) The Design Institute for Physical Properties (DIPPR) Information and Data Evaluation Manager, Version 1.5.0, Copyright BYU -TPL2000.
- (3) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- (4) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- (5) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- (6) Wilson, L.C. 2000. Liquid-Liquid Equilibrium Measurements for Eighteen Glycol Ethers, Ketones, Esters and Alcohols with Water. Project Report No. 44662, 10/13/2000. Union Carbide Corporation, S. Charleston, WV, USA.

10. Summary and Evaluation

Id 123-18-2
Date 18.12.2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT