

# Meprobamate c<sub>9</sub>h<sub>18</sub>n<sub>2</sub>o<sub>4</sub> structure



## Contents

- Retention Index (Linear):

Molecular  
Formula             $C_9H_{18}N_2O_4$

Average mass 218. 250 Da

Density             $1.1 \pm 0.1 \text{ g/cm}^3$

Boiling Point      $434.2 \pm 28.0 \text{ }^\circ\text{C}$  at  
760 mmHg

Flash Point        $229.7 \pm 20.3 \text{ }^\circ\text{C}$

Molar  
Refractivity        $54.3 \pm 0.3 \text{ cm}^3$

Polarizability     $21.5 \pm 0.5 \cdot 10^{-24}$   
 $\text{cm}^3$

Surface  
Tension             $43.9 \pm 3.0 \text{ dyne/cm}$

Molar Volume     $191.5 \pm 3.0 \text{ cm}^3$

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite

- Predicted - ChemAxon
- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

104-106 °C Oxford

University Chemical

Safety Data (No longer

updated) More details

105 °C Jean-Claude

Bradley Open Melting

Point Dataset 15214,

16756, 17165, 21761

104 °C Jean-Claude

Bradley Open Melting

Point Dataset 13021,

8963

97-100

°C LabNetwork LN01295

037

- **Experimental Solubility:**

-1.67Egon

Willighagen [http://dx.](http://dx.doi.org/10.26434/chemrxiv-2015-03-01-10000)

[doi.org/10.](http://dx.doi.org/10.26434/chemrxiv-2015-03-01-10000)

1021/ci050282s

- Miscellaneous

- **Appearance:**

white crystalline

powderOxford

University Chemical

Safety Data (No longer

updated)More details

- **Stability:**

Stable. Combustible.

Incompatible with

strong oxidizing

agents. Oxford

University Chemical

Safety Data (No longer

updated)More details

- **Toxicity:**

IPR-HAM LD50 625 mg

kg-1, ORL-HAM LD50

1410 mg kg-1, IPR-MUS

LD50 331 mg kg-1,

SCU-RAT LD50 525 mg

kg-1Oxford University

Chemical Safety Data

(No longer

updated)More details

- **Safety:**

GHS07BiosynthW-

105461

H302BiosynthW-

105461

Safety glasses,

adequate ventilation.

Oxford University

Chemical Safety Data

(No longer

updated)More details

WarningBiosynthW-

105461

- Gas Chromatography

- **Retention Index (Kovats):**

1652 (estimated with

error: 89)NIST

Spectramainlib\_250606

, replib\_335450,

replib\_10226,  
replib\_221058,  
replib\_246239,  
replib\_312855

1785 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column type: Packed;  
Heat rate: 30 K/min;  
Start T: 100 C; End T:  
310 C; End time: 5 min;  
Start time: 3 min; CAS  
no: 57534; Active  
phase: SE-30; Carrier  
gas: N2; Data type:  
Kovats RI; Authors:  
Maurer, H. H.,  
Identification and  
differentiation of  
barbiturates, other  
sedative-hypnotics and  
their metabolites in  
urine integrated in a  
general screening

procedure using  
computerized gas  
chromatography-mass  
spectrometry, J.

Chromatogr., 530,  
1990, 307-326.)NIST

Spectranist ri

1758 (Program type:  
Isothermal; Col... (show  
more)umn class:

Standard non-polar;

Column diameter: 0. 22  
mm; Column length: 25  
m; Column type:

Capillary; Start T: 200

C; CAS no: 57534;

Active phase: BP-1;

Carrier gas: N2; Phase  
thickness: 0. 25 um;

Data type: Kovats RI;

Authors: Japp, M.; Gill,

R.; Osselton, M. D.,

Comparison of drug

retention indices

determined on packed,

wide bore capillary and  
narrow bore capillary  
columns, J. Forensic  
Sci., 32(6), 1987, 1574-  
1586.)NIST Spectranist  
ri

1764 (Program type:  
Isothermal; Col... (show  
more)umn class:  
Standard non-polar;  
Column diameter: 0. 53  
mm; Column length: 25  
m; Column type:  
Capillary; Start T: 200  
C; CAS no: 57534;  
Active phase: BP-1;  
Carrier gas: N2; Phase  
thickness: 1 um; Data  
type: Kovats RI;  
Authors: Japp, M.; Gill,  
R.; Osselton, M. D.,  
Comparison of drug  
retention indices  
determined on packed,  
wide bore capillary and



narrow bore capillary  
columns, J. Forensic  
Sci., 32(6), 1987, 1574-  
1586.)NIST Spectranist  
ri

1752 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column diameter: 0. 22  
mm; Column length: 12  
m; Column type:  
Capillary; Heat rate: 8  
K/min; Start T: 120 C;  
End T: 300 C; End time:  
12 min; Start time: 2  
min; CAS no: 57534;  
Active phase: SE-30;  
Carrier gas: He; Phase  
thickness: 0. 45 um;  
Data type: Kovats RI;  
Authors: Schepers, P.;  
Wijsbeek, J.; Franke, J.  
P.; de Zeeuw, R. A.,  
Applicability of

capillary gas  
chromatography to  
substance  
identification in  
toxicology by means of  
retention indices, J.  
Forensic Sci., 27(1),  
1982, 49-60.)NIST  
Spectranist ri

1762 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column diameter: 0. 49  
mm; Column length: 25  
m; Column type:  
Capillary; Heat rate: 8  
K/min; Start T: 100 C;  
End T: 275 C; End time:  
15 min; Start time: 2  
min; CAS no: 57534;  
Active phase: SE-30;  
Phase thickness: 1. 14  
um; Data type: Kovats  
RI; Authors: Schepers,

P.; Wijsbeek, J.; Franke,  
J. P.; de Zeeuw, R. A.,  
Applicability of  
capillary gas  
chromatography to  
substance  
identification in  
toxicology by means of  
retention indices, J.  
Forensic Sci., 27(1),  
1982, 49-60.)NIST  
Spectranist ri  
  
1800 (Program type:  
Isothermal; Col... (show  
more)umn class:  
Standard non-polar;  
Column length: 6 ft;  
Column type: Packed;  
CAS no: 57534; Active  
phase: OV-101; Carrier  
gas: N2; Substrate:  
Chromosorb W; Data  
type: Kovats RI;  
Authors: McLinden, V.  
J.; Stenhouse, A. M., A

chromatography  
system for drug  
identification, Forensic  
Sci. Int., 13, 1979, 71-  
79., Program type:  
Isothermal; Col... (show  
more)umn class:  
Standard non-polar;  
Column type: Packed;  
Start T: 200 C; CAS no:  
57534; Active phase:  
OV-1; Data type:  
Kovats RI; Authors:  
Berninger, H.; Moller,  
M. R.,  
Retentionsindices zur  
gaschromatographisch  
en Identifizierung von  
Arzneimitteln, Arch.  
Toxicol., 37, 1977, 295-  
305.)NIST Spectranist ri  
1790 (Program type:  
Isothermal; Col... (show  
more)umn class:  
Standard non-polar;

Column length: 2 m;  
Column type: Packed;  
CAS no: 57534; Active  
phase: SE-30; Data  
type: Kovats RI;  
Authors: Moffat, A. C.;  
Stead, A. H.; Smalldon,  
K. W., Optimum use of  
paper, thin-layer and  
gas-liquid  
chromatography for  
the identification of  
basic drugs. III. Gas-  
liquid chromatography,  
J. Chromatogr., 90,  
1974, 19-33.)NIST  
Spectranist ri

- **Retention Index (Lee):**

301. 69 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column type: Capillary;  
CAS no: 57534; Active  
phase: Methyl Silicone;

Data type: Lee RI;  
Authors: Eckel, W. P.;  
Ross, B.; Isensee, R. K.,  
Pentobarbital found in  
ground water, Ground  
Water, 31(5), 1993,  
801-804.)NIST  
Spectranist ri

304. 55 (Program type:  
Ramp; Column cl...  
(show more)ass:

Standard non-polar;  
Column type: Capillary;  
CAS no: 57534; Active  
phase: Methyl Silicone;  
Data type: Lee RI;  
Authors: Eckel, W. P.;  
Ross, B.; Isensee, R. K.,  
Pentobarbital found in  
ground water, Ground  
Water, 31(5), 1993,  
801-804.)NIST  
Spectranist ri

- **Retention Index (Normal Alkane):**

1771 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column diameter: 0. 26

mm; Column length: 30

m; Column type:

Capillary; Heat rate: 8

K/min; Start T: 120 C;

End T: 280 C; End time:

22 min; Start time: 1

min; CAS no: 57534;

Active phase: DB-1;

Carrier gas: He; Phase

thickness: 0. 25 um;

Data type: Normal

alkane RI; Authors:

Manca, D.; Ferron, L.;

Weber, J-P., A System

for Toxicological

Screening by Capillary

Gas Chromatography

with Use of Drug

Retention Index Based

on Nitrogen-Containing

Reference Compounds,  
Clin. Chem., 35(4),  
1989, 601-607.)NIST  
Spectranist ri  
  
1750 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column diameter: 0. 53  
mm; Column length: 10  
m; Column type:  
Capillary; Heat rate: 5  
K/min; Start T: 130 C;  
End T: 230 C; CAS no:  
57534; Active phase:  
DB-1; Carrier gas: He;  
Phase thickness: 2. 65  
um; Data type: Normal  
alkane RI; Authors:  
Anderson, W. H.; Fuller,  
D. C., A simplified  
procedure for the  
isolation,  
characterization, and  
identification of weak



acid and neutral drugs  
from whole blood, J.  
Anal. Toxicol., 11,  
1987, 198-204.)NIST  
Spectranist ri  
  
1758 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column diameter: 0. 25  
mm; Column length: 15  
m; Column type:  
Capillary; Heat rate: 10  
K/min; Start T: 130 C;  
End T: 290 C; End time:  
10 min; Start time: 1  
min; CAS no: 57534;  
Active phase: DB-1;  
Carrier gas: He; Phase  
thickness: 0. 25 um;  
Data type: Normal  
alkane RI; Authors:  
Sharp, M. E., A rapid  
screening procedure  
for acidic and neutral

drugs in blood by high  
resolution gas  
chromatography, J.  
Anal. Toxicol., 11,  
1987, 8-11.)NIST  
Spectranist ri

1810 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column length: 2 m;  
Column type: Packed;  
Heat rate: 2.5 K/min;  
Start T: 120 C; End T:  
200 C; CAS no: 57534;  
Active phase: OV-1;  
Substrate: Gas Chrom  
P; Data type: Normal  
alkane RI; Authors:  
Marozzi, E.; Gambaro,  
V.; Saligari, E.; Mariani,  
R.; Lodi, F., Use of the  
retention index in gas  
chromatographic  
studies of drugs, J.

Anal. Toxicol., 6, 1982,  
185-192., Program  
type: Ramp; Column  
cl... (show more)ass:  
Standard non-polar;  
Column length: 2 m;  
Column type: Packed;  
Heat rate: 2.5 K/min;  
Start T: 120 C; End T:  
200 C; CAS no: 57534;  
Active phase: SE-30;  
Substrate: Gas Chrom  
P; Data type: Normal  
alkane RI; Authors:  
Marozzi, E.; Gambaro,  
V.; Saligari, E.; Mariani,  
R.; Lodi, F., Use of the  
retention index in gas  
chromatographic  
studies of drugs, J.  
Anal. Toxicol., 6, 1982,  
185-192.)NIST  
Spectranist ri  
1796 (Program type:  
Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column type: Other;

CAS no: 57534; Active

phase: Methyl Silicone;

Data type: Normal

alkane RI; Authors:

Ardrey, R. E.; Moffat, A.

C., Gas-liquid

chromatographic

retention indices of

1318 substances of

toxicological interest

on SE-30 or OV-1

stationary phase, J.

Chromatogr., 220,

1981, 195-252.)NIST

Spectranist ri

1785 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column length: 6 ft;

Column type: Packed;

Heat rate: 8 K/min;

Start T: 130 C; End T:  
290 C; End time: 8 min;  
Start time: 2 min; CAS  
no: 57534; Active  
phase: SE-30; Carrier  
gas: N2; Substrate:  
Chromosorb W AW  
DMS; Data type:  
Normal alkane RI;  
Authors: Peel, H. W.;  
Perrigo, B., A practical  
gas chromatographic  
screening procedure  
for toxicological  
analysis, Can. Soc.  
Forens. Sci. J., 9(2),  
1975, 69-74., Program  
type: Ramp; Column  
cl... (show more)ass:  
Standard non-polar;  
Column length: 6 ft;  
Column type: Packed;  
Heat rate: 8 K/min;  
Start T: 130 C; End T:  
290 C; End time: 8 min;  
Start time: 2 min; CAS

no: 57534; Active

phase: SE-30; Carrier

gas: Nitrogen;

Substrate: Chromosorb

W AW DMS (80-100

mesh); Data type:

Normal alkane RI;

Authors: Peel, H. W.;

Perrigo, B., A practical

gas chromatographic

screening procedure

for toxicological

analysis, Can. Soc.

Forens. Sci. J., 9(2),

1976, 69-74.)NIST

Spectranist ri

1830 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column length: 6 ft;

Column type: Packed;

Heat rate: 8 K/min;

Start T: 130 C; End T:

290 C; End time: 8 min;

Start time: 2 min; CAS  
no: 57534; Active  
phase: SE-30; Carrier  
gas: N2; Substrate:  
Chromosorb W AW  
DMS; Data type:  
Normal alkane RI;  
Authors: Peel, H. W.;  
Perrigo, B., A practical  
gas chromatographic  
screening procedure  
for toxicological  
analysis, Can. Soc.  
Forens. Sci. J., 9(2),  
1975, 69-74., Program  
type: Ramp; Column  
cl... (show more)ass:  
Standard non-polar;  
Column length: 6 ft;  
Column type: Packed;  
Heat rate: 8 K/min;  
Start T: 130 C; End T:  
290 C; End time: 8 min;  
Start time: 2 min; CAS  
no: 57534; Active  
phase: SE-30; Carrier

gas: Nitrogen;

Substrate: Chromosorb

W AW DMS (80-100

mesh); Data type:

Normal alkane RI;

Authors: Peel, H. W.;

Perrigo, B., A practical

gas chromatographic

screening procedure

for toxicological

analysis, Can. Soc.

Forens. Sci. J., 9(2),

1976, 69-74.)NIST

Spectranist ri

1826 (Program type:

Complex; Column...

(show more)class:

Semi-standard non-

polar; Column

diameter: 0. 20 mm;

Column length: 25 m;

Column type: Capillary;

Description: 50 0C (0. 5

min) ^ 99 0C/min ->

100 0C (1 min) ^ 15



0C/min -> 280 0C (20  
min); CAS no: 57534;  
Active phase: 5 %  
Phenyl methyl siloxane;  
Phase thickness: 0.33  
um; Data type: Normal  
alkane RI; Authors:  
Grigoriev, A. M.;  
Savchuk, S. A.,  
Correlation of the  
parameters of  
screening libraries of  
the gas-  
chromatographic  
retention data, Rus. J.  
Anal. Chem. (Engl.  
Transl.), 65(4), 2010,  
388-397, In original  
400-409.)NIST  
Spectranist ri  
1832 (Program type:  
Complex; Column...  
(show more)class:  
Semi-standard non-  
polar; Column

diameter: 0.20 mm;  
Column length: 25 m;  
Column type: Capillary;  
Description: 50 °C (0.5  
min) ^ 99 °C/min ->  
100 °C (1 min) ^ 15  
°C/min -> 280 °C (20  
min); CAS no: 57534;  
Active phase: 5 %  
Phenyl methyl siloxane;  
Phase thickness: 0.33  
µm; Data type: Normal  
alkane RI; Authors:  
Grigoriev, A. M.;  
Savchuk, S. A.,  
Correlation of the  
parameters of  
screening libraries of  
the gas-  
chromatographic  
retention data, Rus. J.  
Anal. Chem. (Engl.  
Transl.), 65(4), 2010,  
388-397, In original  
400-409.)NIST

Spectranist ri

1802. 5 (Program type:

Ramp; Column cl...

(show more)ass: Semi-

standard non-polar;

Column diameter: 0. 32

mm; Column length:

12. 5 m; Column type:

Capillary; Heat rate: 10

K/min; Start T: 110 C;

End T: 290 C; End time:

6. 5 min; Start time: 1

min; CAS no: 57534;

Active phase: Ultra-2;

Phase thickness: 0. 5

um; Data type: Normal

alkane RI; Authors:

Watts, V. W.; Simonick,

T. F., A retention index

library for commonly

encountered drugs and

metabolites using tri-n-

alkylamines as

reference compounds,

nitrogen-phosphorus

detectors, and dual  
capillary  
chromatography, J.  
Anal. Toxicol., 11,  
1987, 210-214.)NIST  
Spectranist ri

- **Retention Index (Linear):**

1784 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column diameter: 0. 75  
mm; Column length: 30  
m; Column type:  
Capillary; Heat rate: 10  
K/min; Start T: 160 C;  
End T: 280 C; End time:  
12 min; CAS no: 57534;  
Active phase: SPB-1;  
Carrier gas: He; Phase  
thickness: 1. 0 um;  
Data type: Linear RI;  
Authors: Christ, D. W.;  
Noomano, P.; Rosas,  
M.; Rhone, D.,

Retention indices by  
wide-bore capillary gas  
chromatography with  
nitrogen-phosphorus  
detection, J. Anal.

Toxicol., 12, 1988, 84-  
88.)NIST Spectranist ri

1762 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column diameter: 0. 25

mm; Column length: 15

m; Column type:

Capillary; Heat rate: 8

K/min; Start T: 120 C;

End T: 280 C; End time:

5 min; CAS no: 57534;

Active phase: DB-1;

Carrier gas: He; Phase

thickness: 0. 25 um;

Data type: Linear RI;

Authors: Perrigo, B. J.;

Ballantyne, D. J.; Peel,

H. W., Condierations in

developing a data base  
for drugs on a DBI  
capillary column, J.  
Can. Soc. Forensic Sci.,  
17(2), 1984, 41-49.,  
Program type: Ramp;  
Column cl... (show  
more)ass: Standard  
non-polar; Column  
diameter: 0. 32 mm;  
Column length: 15 m;  
Column type: Capillary;  
Heat rate: 8 K/min;  
Start T: 120 C; End T:  
280 C; End time: 5 min;  
CAS no: 57534; Active  
phase: DB-1; Carrier  
gas: He; Phase  
thickness: 0. 25 um;  
Data type: Linear RI;  
Authors: Perrigo, B. J.;  
Peel, H. W.; Ballantyne,  
D. J., Use of Dual-  
Column Fused-Silica  
Capillary Gas  
Chromatography in

Combination with  
Detector Response  
Factors for Analytical  
Toxicology., J.  
Chromatogr., 341,  
1985, 81-88.)NIST  
Spectranist ri

1758 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column diameter: 0. 2  
mm; Column length: 12  
m; Column type:  
Capillary; Heat rate: 20  
K/min; Start T: 50 C;  
End T: 300 C; End time:  
3 min; Start time: 1  
min; CAS no: 57534;  
Active phase: Methyl  
Silicone; Carrier gas:  
He; Phase thickness: 0.  
33 um; Data type:  
Linear RI; Authors:  
Newton, B.; Foery, R.

F., Retention indices  
and dual capillary gas  
chromatography for  
rapid identification of  
sedative hypnotic  
drugs in emergency  
toxicology, J. Anal.  
Toxicol., 8, 1984, 129-  
134.)NIST Spectranist ri

1780 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column length: 1. 8 m;  
Column type: Packed;  
Heat rate: 8 K/min;  
Start T: 130 C; End T:  
290 C; End time: 8 min;  
Start time: 2 min; CAS  
no: 57534; Active  
phase: SE-30; Carrier  
gas: N2; Substrate:  
Chromosorb W; Data  
type: Linear RI;  
Authors: Perrigo, B. J.;



Peel, H. W., The use of retention indices and temperature-programmed gas chromatography in analytical toxicology, J. Chromatogr. Sci., 19, 1981, 219-226.)NIST Spectranist ri

Predicted data is generated using the ACD/Labs Percepta Platform - PhysChem Module

Density:	1.1 ± 0.1 g/cm <sup>3</sup>
Boiling Point:	434.2 ± 28.0 °C at 760 mmHg
Vapour Pressure:	0.0 ± 1.0 mmHg at 25°C
Enthalpy of Vaporization:	69.0 ± 3.0 kJ/mol
Flash Point:	229.7 ± 20.3 °C
Index of Refraction:	1.479
Molar Refractivity:	54.3 ± 0.3 cm <sup>3</sup>
#H bond acceptors:	6
#H bond donors:	4

#Freely Rotating Bonds:	8
#Rule of 5 Violations:	0
ACD/LogP:	0.70
ACD/LogD (pH 5.5):	0.82
ACD/BCF (pH 5.5):	2.49
ACD/KOC (pH 5.5):	66.88
ACD/LogD (pH 7.4):	0.82
ACD/BCF (pH 7.4):	2.49
ACD/KOC (pH 7.4):	66.88
Polar Surface Area:	105 Å <sup>2</sup>
Polarizability:	21.5 ± 0.5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	43.9 ± 3.0 dyne/cm
Molar Volume:	191.5 ± 3.0 cm <sup>3</sup>

Predicted data is generated using the US Environmental Protection Agency's EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 0. 98Log Kow (Exper. database match) = 0. 70Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 282. 95 (Adapted Stein & Brown method)Melting Pt (deg C): 46. 59 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 000792 (Modified Grain method)MP (exp database): 105 deg CSubcooled liquid VP: 0. 0048 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 8877log Kow used: 0. 70 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 4700 mg/L (25 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 9764. 7 mg/LWat Sol (Exper. database match) = 4700. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 85E-010 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 562E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 70 (exp database)Log Kaw used: -8. 121 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 8. 821Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6188Biowin2 (Non-Linear Model) : 0. 5511Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 4113 (weeks-months)Biowin4 (Primary Survey Model) : 3. 7667 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2420Biowin6 (MITI Non-Linear Model): 0. 3140Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 4467Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 64 Pa (0. 0048 mm Hg)Log Koa (Koawin est ) : 8. 821Kp (particle/gas partition coef. (m3/ug)): Mackay model : 4. 69E-006 Octanol/air (Koa) model: 0. 000163 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000169 Mackay model : 0. 000375 Octanol/air (Koa) model: 0. 0128 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 19. 3251 E-12 cm3/molecule-secHalf-Life = 0. 553 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 6. 642 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000272 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 173. 4Log Koc: 2. 239 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 1. 320E-004 L/mol-secKb Half-Life at pH 8: 166. 327 years Kb Half-Life at pH 7: 1663. 267 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0. 500 (BCF = 3. 162)log Kow used: 0. 70 (expkow database)Volatilization from Water: Henry LC: 1. 85E-010 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 4. 675E+006 hours (1. 948E+005 days)Half-Life from Model Lake : 5. 1E+007 hours (2. 125E+006 days)Removal In Wastewater Treatment: Total removal: 1. 87 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 77 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 00248 13. 3 1000 Water 43. 3 900 1000 Soil 56. 6 1. 8e+003 1000 Sediment 0. 0873 8. 1e+003 0 Persistence Time: 1. 01e+003 hr

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