

1-propylcyclohexene  
c<sub>9</sub>h<sub>16</sub> structure



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## Contents

- Retention Index (Normal Alkane):

Molecular Formula	C <sub>9</sub> H <sub>16</sub>
Average mass	124. 223 Da
Density	0. 8±0. 1 g/cm <sup>3</sup>
Boiling Point	159. 2±7. 0 °C at 760 mmHg
Flash Point	36. 4±6. 6 °C
Molar Refractivity	41. 2±0. 3 cm <sup>3</sup>
Polarizability	16. 3±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension	26. 6±3. 0 dyne/cm
Molar Volume	151. 8±3. 0 cm <sup>3</sup>

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Gas Chromatography

- **Retention Index (Kovats):**

990 (estimated with error: 39)NIST Spectramainlib\_142689

944 (Program type: Isothermal; Col... (show more)umn class: Semi-stand  
polar; Column diameter: 0. 25 mm; Column length: 80 m; Column type: C  
Start T: 60 C; CAS no: 2539755; Active phase: Squalane; Data type: Kova  
Authors: Orav, A.; Eisen, O., The retention indexes for alkenes, alkynes a  
cyclenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(  
1972, 39-47., Program type: Isothermal; Col... (show more)umn class: Se  
standard non-polar; Column type: Packed; Start T: 60 C; CAS no: 253975  
phase: Squalane; Data type: Kovats RI; Authors: Bogoslovsky, Yu. N.; Anv  
I.; Vigdergauz, M. S., Chromatographic constants in gas chromatography  
Russian), Standards Publ. House, Moscow, 1978, 192.)NIST Spectranist ri

949 (Program type: Isothermal; Col... (show more)umn class: Semi-stand  
polar; Column type: Packed; Start T: 80 C; CAS no: 2539755; Active phas  
Squalane; Data type: Kovats RI; Authors: Bogoslovsky, Yu. N.; Anvaer, B.  
Vigdergauz, M. S., Chromatographic constants in gas chromatography (in  
Russian), Standards Publ. House, Moscow, 1978, 192.)NIST Spectranist ri

954 (Program type: Isothermal; Col... (show more)umn class: Semi-stand  
polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type:  
Capillary; Start T: 100 C; CAS no: 2539755; Active phase: Squalane; Carr  
Nitrogen or helium; Data type: Kovats RI; Authors: Rang, S.; Orav, A.; Kur  
K.; Eisen, O., Capillary Gas Chromatography of Monosubstituted Cycloper  
and Cyclohexenes, Chromatographia, 10(3), 1977, 115-122.)NIST Spectr

944. 5 (Program type: Isothermal; Col... (show more)umn class: Semi-sta  
non-polar; Column diameter: 0. 25 mm; Column length: 80 m; Column ty  
Capillary; Start T: 60 C; CAS no: 2539755; Active phase: Squalane; Data  
Kovats RI; Authors: Eisen, O.; Orav, A.; Rang, S., Identifizierung von Norm  
Alkenen, Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatogra  
Identification des alcenes, cyclopentenes et -hexenes a l'aide de la  
chromatographie en phase gazeuse sur colonne capillaire, Chromatograph  
1972, 229-239.)NIST Spectranist ri

949. 6 (Program type: Isothermal; Col... (show more)umn class: Semi-sta  
non-polar; Column diameter: 0. 25 mm; Column length: 80 m; Column ty  
Capillary; Start T: 80 C; CAS no: 2539755; Active phase: Squalane; Data  
Kovats RI; Authors: Eisen, O.; Orav, A.; Rang, S., Identifizierung von Norm  
Alkenen, Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatogra  
Identification des alcenes, cyclopentenes et -hexenes a l'aide de la  
chromatographie en phase gazeuse sur colonne capillaire, Chromatograph  
1972, 229-239.)NIST Spectranist ri

979 (Program type: Isothermal; Col... (show more)umn class: Semi-stand  
polar; Column diameter: 0. 25 mm; Column length: 45 m; Column type: C  
Start T: 100 C; CAS no: 2539755; Active phase: Apiezon L; Data type: Ko  
Authors: Eisen, O.; Orav, A.; Rang, S., Identifizierung von Normal-Alkenen  
Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatographie.  
Identification des alcenes, cyclopentenes et -hexenes a l'aide de la  
chromatographie en phase gazeuse sur colonne capillaire, Chromatograph

1972, 229-239.)NIST Spectranist ri

988 (Program type: Isothermal; Col... (show more)umn class: Semi-stand  
polar; Column diameter: 0. 25 mm; Column length: 45 m; Column type: C  
Start T: 120 C; CAS no: 2539755; Active phase: Apiezon L; Data type: Ko  
Authors: Eisen, O.; Orav, A.; Rang, S., Identifizierung von Normal-Alkener  
Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatographie.  
Identification des alcenes, cyclopentenes et -hexenes a l'aide de la  
chromatogrphie en phase gazeuse sur colonne capillaire, Chromatograp  
1972, 229-239.)NIST Spectranist ri

950 (Program type: Isothermal; Col... (show more)umn class: Semi-stand  
polar; Column diameter: 0. 25 mm; Column length: 80 m; Column type: C  
Start T: 80 C; CAS no: 2539755; Active phase: Squalane; Data type: Kova  
Authors: Orav, A.; Eisen, O., The retention indexes for alkenes, alkynes a  
cyclenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(  
1972, 39-47.)NIST Spectranist ri

1076 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column type: Capillary; Start T: 80 C; CAS no: 2539755; Active phase: PE  
Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; M  
A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics o  
unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn,  
SSR, 1988, 208.)NIST Spectranist ri

1079 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column diameter: 0. 25 mm; Column length: 80 m; Column type: Capilla

T: 60 C; CAS no: 2539755; Active phase: PEG 4000; Data type: Kovats RI  
Authors: Orav, A.; Eisen, O., The retention indexes for alkenes, alkynes and  
cyclohexenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(1972),  
1972, 39-47., Program type: Isothermal; Column class: Standard  
polar; Column type: Capillary; Start T: 60 C; CAS no: 2539755; Active phase:  
4000; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K.  
Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics  
of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn,  
Estonia SSR, 1988, 208.)NIST Spectranist ri

1081 (Program type: Isothermal; Column class: Standard  
Column type: Capillary; Start T: 90 C; CAS no: 2539755; Active phase: PE  
Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; M  
A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of  
unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn,  
SSR, 1988, 208.)NIST Spectranist ri

1086 (Program type: Isothermal; Column class: Standard  
Column type: Capillary; Start T: 100 C; CAS no: 2539755; Active phase: P  
Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; M  
A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of  
unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn,  
SSR, 1988, 208.)NIST Spectranist ri

1090 (Program type: Isothermal; Column class: Standard  
Column type: Capillary; Start T: 80 C; CAS no: 2539755; Active phase: PE  
Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; M

A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208.)NIST Spectranist ri

1091 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column type: Capillary; Start T: 110 C; CAS no: 2539755; Active phase: PEG-20M; Carrier gas: Helium; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208.)NIST Spectranist ri

1094 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column diameter: 0.25 mm; Column length: 100 m; Column type: Capillary; Start T: 120 C; CAS no: 2539755; Active phase: PEG-20M; Carrier gas: Helium; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary chromatography of monosubstituted cyclopentenes and cyclohexenes on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-43.)NIST Spectranist ri  
1100 (Program type: Isothermal; Col... (show more)umn class: Standard polar;  
Column type: Capillary; Start T: 120 C; CAS no: 2539755; Active phase: PEG-20M; Carrier gas: Helium; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208.)NIST Spectranist ri

1100 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column diameter: 0.25 mm; Column length: 45 m; Column type: Capillary; Start T: 100 C; CAS no: 2539755; Active phase: PEG 4000; Carrier gas: Nitrogen; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208.)NIST Spectranist ri

Helium; Data type: Kovats RI; Authors: Rang, S.; Orav, A.; Kuningas, K.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons. In: Proceedings of the Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208. JN15  
 Capillary Gas Chromatography of Monosubstituted Cyclopentenes and Cyclohexenes, Chromatographia, 10(3), 1977, 115-122., Program type: Isothermal; Column class: Standard polar; Column type: Capillary  
 Start T: 100 C; CAS no: 2539755; Active phase: PEG 4000; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, A.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons. In: Proceedings of the Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208. JN15  
 Spectranist ri

1075. 8 (Program type: Isothermal; Column class: Standard polar; Column type: Capillary  
 Column diameter: 0.25 mm; Column length: 100 m; Column type: Capillary  
 Start T: 80 C; CAS no: 2539755; Active phase: PEG-20M; Carrier gas: Helium; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of monosubstituted cyclopentenes and cyclohexenes on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-45.  
 Spectranist ri

1081. 4 (Program type: Isothermal; Column class: Standard polar; Column type: Capillary  
 Column diameter: 0.25 mm; Column length: 100 m; Column type: Capillary  
 Start T: 90 C; CAS no: 2539755; Active phase: PEG-20M; Carrier gas: Helium; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of monosubstituted cyclopentenes and cyclohexenes on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-45.  
 Spectranist ri

1086. 4 (Program type: Isothermal; Column class: Standard polar; Column type: Capillary



Column diameter: 0.25 mm; Column length: 100 m; Column type: Capillary  
Start T: 100 C; CAS no: 2539755; Active phase: PEG-20M; Carrier gas: Helium  
Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary  
gas chromatography of monosubstituted cyclopentenes and cyclohexenes  
on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-43  
NIST Spectranist ri

1090. 8 (Program type: Isothermal; Column class: Standard)  
Column diameter: 0.25 mm; Column length: 100 m; Column type: Capillary  
Start T: 110 C; CAS no: 2539755; Active phase: PEG-20M; Carrier gas: Helium  
Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary  
gas chromatography of monosubstituted cyclopentenes and cyclohexenes  
on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-43  
NIST Spectranist ri

1079. 3 (Program type: Isothermal; Column class: Standard)  
Column diameter: 0.25 mm; Column length: 80 m; Column type: Capillary  
Start T: 60 C; CAS no: 2539755; Active phase: Polyethylene Glycol 4000; Data  
type: Kovats RI; Authors: Eisen, O.; Orav, A.; Rang, S., Identifizierung von Normalk  
Alkenen, Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatographie  
Identification des alcenes, cyclopentenes et -hexenes a l'aide de la  
chromatographie en phase gazeuse sur colonne capillaire, Chromatographica  
1972, 229-239.)NIST Spectranist ri

1090. 2 (Program type: Isothermal; Column class: Standard)  
Column diameter: 0.25 mm; Column length: 80 m; Column type: Capillary  
Start T: 80 C; CAS no: 2539755; Active phase: PEG 4000; Data type: Kovats RI

Authors: Orav, A.; Eisen, O., The retention indexes for alkenes, alkynes and cycloalkenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(1972), 39-47., Program type: Isothermal; Column class: Standard; Column polarity: Non-polar; Column diameter: 0.25 mm; Column length: 80 m; Column type: Capillary; Start T: 80 C; CAS no: 2539755; Active phase: Polyethylene Glycol 4000; Data type: Kovats RI; Authors: Eisen, O.; Orav, A.; Rang, S., Identifizierung von Alkenen, Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatographie. Identification des alcenes, cyclopentenes et -hexenes a l'aide de la chromatographie en phase gazeuse sur colonne capillaire, Chromatographia 1972, 229-239.)NIST Spectranist ri

1099. 6 (Program type: Isothermal; Column class: Standard; Column polarity: Non-polar; Column diameter: 0.25 mm; Column length: 80 m; Column type: Capillary; Start T: 100 C; CAS no: 2539755; Active phase: PEG 4000; Data type: Kovats RI; Authors: Orav, A.; Eisen, O., The retention indexes for alkenes, alkynes and cycloalkenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(1972), 39-47., Program type: Isothermal; Column class: Standard; Column polarity: Non-polar; Column diameter: 0.25 mm; Column length: 80 m; Column type: Capillary; Start T: 100 C; CAS no: 2539755; Active phase: Polyethylene Glycol 4000; Data type: Kovats RI; Authors: Eisen, O.; Orav, A.; Rang, S., Identifizierung von Alkenen, Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatographie. Identification des alcenes, cyclopentenes et -hexenes a l'aide de la chromatographie en phase gazeuse sur colonne capillaire, Chromatographia 1972, 229-239.)NIST Spectranist ri

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

965 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 2539755; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Zenkevich, I. G., Mutual Correlation between Gas Chromatographic Retention Indices of Unsaturated and Saturated Hydrocarbons found by Molecular Dynamics, Z. Anal. Chem., 55(10), 2000-1097, In original 1091-1097.)NIST Spectranist ri

952 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0.26 mm; Column length: 52 m; Column type: Capillary; Flow rate: 3 K/min; Start T: 50 C; End T: 220 C; CAS no: 2539755; Active phase: 101; Carrier gas: N2; Data type: Normal alkane RI; Authors: Chupalov, A., Zenkevich, I. G., Chromatographic Characterization of Structural Transformations of Organic Compounds in Diels-Alder Reaction. Aliphatic Dienes and Dienophiles, Zh. Org. Khim., 32(6), 1996, 675-684, In original 675-684.)NIST Spectranist ri

938 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Flow rate: 4 K/min; Start T: 40 C; End T: 250 C; CAS no: 2539755; Active phase: 2100; Carrier gas: He; Data type: Normal alkane RI; Authors: Alencar, J. V., Alves, P. B.; Craveiro, A. A., Pyrolysis of tropical vegetable oils, J. Agric. Food Chem., 31, 1983, 1268-1270.)NIST Spectranist ri

944 (Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 2539755; Active phase: Squalane; Data type: Normal alkane RI; Authors: Chen, H.-F., Quantitative prediction of gas chromatography retention indices with support vector machines, radial basis

neutral networks and multiple linear regression, Anal. Chim. Acta, 609, 2

36.)NIST Spectranist ri

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

Density:	0.8±0.1 g/cm <sup>3</sup>
Boiling Point:	159.2±7.0 °C at 760 mmHg
Vapour Pressure:	3.3±0.1 mmHg at 25°C
Enthalpy of Vaporization:	38.0±0.8 kJ/mol
Flash Point:	36.4±6.6 °C
Index of Refraction:	1.455
Molar Refractivity:	41.2±0.3 cm <sup>3</sup>
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0
ACD/LogP:	4.55
ACD/LogD (pH 5.5):	4.08

ACD/BCF (pH 5. 5):	743. 67
ACD/KOC (pH 5. 5):	3953. 10
ACD/LogD (pH 7. 4):	4. 08
ACD/BCF (pH 7. 4):	743. 67
ACD/KOC (pH 7. 4):	3953. 10
Polar Surface Area:	0 Å <sup>2</sup>
Polarizability:	16. 3±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	26. 6±3. 0 dyne/cm
Molar Volume:	151. 8±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) = 4. 49  
Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42):  
Boiling Pt (deg C): 159. 86 (Adapted Stein & Brown method) Melting Pt (deg C):  
-38. 69 (Mean or Weighted MP) VP (mm Hg, 25 deg C): 3. 31 (Mean VP of Antoine &  
Grain methods) Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water  
Solubility at 25 deg C (mg/L): 4. 114 log Kow used: 4. 49 (estimated) no-  
melting pt equation used Water Sol Estimate from Fragments: Wat Sol (v1. 01  
est) = 11. 045 mg/L ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found:  
Neutral Organics Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method  
: 1. 83E-001 atm-m<sup>3</sup>/mole Group Method: 1. 81E-001 atm-m<sup>3</sup>/mole Henrys LC  
[VP/WSol estimate using EPI values]: 1. 315E-001 atm-m<sup>3</sup>/mole Log Octanol-Air  
Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 49 (KowWin  
est) Log Kaw used: 0. 874 (HenryWin est) Log Koa (KOAWIN v1. 10 estimate): 3.  
616 Log Koa (experimental database): None Probability of Rapid Biodegradation  
(BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6884 Biowin2 (Non-Linear Model) :  
0. 7764 Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model):

<https://assignbuster.com/1-propylcyclohexene-c9h16-structure/>

2. 9246 (weeks )Biowin4 (Primary Survey Model) : 3. 6685 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5269Biowin6 (MITI Non-Linear Model): 0. 6883Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2549Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 0. 8741BioHC Half-Life (days) : 7. 4838Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 404 Pa (3. 03 mm Hg)Log Koa (Koawin est ): 3. 616Kp (particle/gas partition coef. (m3/ug)): Mackay model : 7. 43E-009 Octanol/air (Koa) model: 1. 01E-009 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 68E-007 Mackay model : 5. 94E-007 Octanol/air (Koa) model: 8. 11E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 94. 4887 E-12 cm3/mole-secHalf-Life = 0. 113 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 358 HrsOzone Reaction: OVERALL Ozone Rate Constant = 43. 000000 E-17 cm3/mole-secHalf-Life = 0. 027 Days (at 7E11 mol/cm3)Half-Life = 38. 378 MinReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 4. 31E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 955Log Koc: 2. 980 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Rate constants can NOT be estimated for this structure! Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 2. 757 (BCF = 572)log Kow used: 4. 49 (estimated)Volatilization from Water: Henry LC: 0. 183 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 141 hoursHalf-Life from Model Lake : 105. 9 hours (4. 413 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 98. 97 percentTotal biodegradation: 0. 11 percentTotal sludge adsorption: 33. 55 percentTotal to Air: 65. 30 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 293 0. 518 1000 Water 33. 5 360 1000 Soil 53. 7 720 1000 Sediment 12. 5 3. 24e+003 0 Persistence Time: 182 hr

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