

# [1-propylcyclohexene c9h16 structure](https://assignbuster.com/1-propylcyclohexene-c9h16-structure/)

Contents

* Retention Index (Normal Alkane):

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

* 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-standard non-polar; Column diameter: 0. 25 mm; Column length: 80 m; Column type: Capillary; Start T: 60 C; CAS no: 2539755; Active phase: Squalane; Data type: Kovats RI; Authors: Orav, A.; Eisen, O., The retention indexes for alkenes, alkynes and cyclenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(1), 1972, 39-47., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 60 C; CAS no: 2539755; Active phase: Squalane; Data type: Kovats RI; Authors: Bogoslovsky, Yu. N.; Anvaer, B. I.; Vigdergauz, M. S., Chromatographic constants in gas chromatography (in Russian), Standards Publ. House, Moscow, 1978, 192.)NIST Spectranist ri  |
| 949 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 80 C; CAS no: 2539755; Active phase: Squalane; Data type: Kovats RI; Authors: Bogoslovsky, Yu. N.; Anvaer, B. I.; 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-standard non-polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 100 C; CAS no: 2539755; Active phase: Squalane; Carrier gas: Nitrogen or helium; Data type: Kovats RI; Authors: Rang, S.; Orav, A.; Kuningas, K.; Eisen, O., Capillary Gas Chromatography of Monosubstituted Cyclopentenes and Cyclohexenes, Chromatographia, 10(3), 1977, 115-122.)NIST Spectranist ri  |
| 944. 5 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 80 m; Column type: Capillary; Start T: 60 C; CAS no: 2539755; Active phase: Squalane; Data type: Kovats RI; 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 chromatogrpahie en phase gazeuse sur colonne capillaire, Chromatographia, 5, 1972, 229-239.)NIST Spectranist ri  |
| 949. 6 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 80 m; Column type: Capillary; Start T: 80 C; CAS no: 2539755; Active phase: Squalane; Data type: Kovats RI; 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 chromatogrpahie en phase gazeuse sur colonne capillaire, Chromatographia, 5, 1972, 229-239.)NIST Spectranist ri  |
| 979 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 45 m; Column type: Capillary; Start T: 100 C; CAS no: 2539755; Active phase: Apiezon L; Data type: Kovats RI; 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 chromatogrpahie en phase gazeuse sur colonne capillaire, Chromatographia, 5, 1972, 229-239.)NIST Spectranist ri  |
| 988 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 45 m; Column type: Capillary; Start T: 120 C; CAS no: 2539755; Active phase: Apiezon L; Data type: Kovats RI; 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 chromatogrpahie en phase gazeuse sur colonne capillaire, Chromatographia, 5, 1972, 229-239.)NIST Spectranist ri  |
| 950 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 80 m; Column type: Capillary; Start T: 80 C; CAS no: 2539755; Active phase: Squalane; Data type: Kovats RI; Authors: Orav, A.; Eisen, O., The retention indexes for alkenes, alkynes and cyclenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(1), 1972, 39-47.)NIST Spectranist ri  |
| 1076 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 80 C; CAS no: 2539755; Active phase: PEG-20M; 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  |
| 1079 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 80 m; Column type: Capillary; Start 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 cyclenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(1), 1972, 39-47., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 60 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, 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; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 90 C; CAS no: 2539755; Active phase: PEG-20M; 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  |
| 1086 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 100 C; CAS no: 2539755; Active phase: PEG-20M; 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  |
| 1090 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 80 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, 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 polar; Column type: Capillary; Start T: 110 C; CAS no: 2539755; Active phase: PEG-20M; 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 polar; 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: He; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of monosubstituted cyclopentenes and cyclohexenes C8-C15 on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-49., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 120 C; CAS no: 2539755; Active phase: PEG-20M; 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 polar; 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 or Helium; Data type: Kovats RI; Authors: Rang, S.; Orav, A.; Kuningas, K.; Eisen, O., Capillary Gas Chromatography of Monosubstituted Cyclopentenes and Cyclohexenes, Chromatographia, 10(3), 1977, 115-122., Program type: Isothermal; Col… (show more)umn 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, 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  |
| 1075. 8 (Program type: Isothermal; Col… (show more)umn class: Standard polar; 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: He; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of monosubstituted cyclopentenes and cyclohexenes C8-C15 on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-49.)NIST Spectranist ri  |
| 1081. 4 (Program type: Isothermal; Col… (show more)umn class: Standard polar; 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: He; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of monosubstituted cyclopentenes and cyclohexenes C8-C15 on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-49.)NIST Spectranist ri  |
| 1086. 4 (Program type: Isothermal; Col… (show more)umn class: Standard polar; 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: He; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of monosubstituted cyclopentenes and cyclohexenes C8-C15 on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-49.)NIST Spectranist ri  |
| 1090. 8 (Program type: Isothermal; Col… (show more)umn class: Standard polar; 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: He; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of monosubstituted cyclopentenes and cyclohexenes C8-C15 on polyethylene glycol 20M, Eesti NSV Tead. Akad. Toim. Keem., , 1982, 40-49.)NIST Spectranist ri  |
| 1079. 3 (Program type: Isothermal; Col… (show more)umn class: Standard polar; 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 Normal-Alkenen, Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatographie. Identification des alcenes, cyclopentenes et -hexenes a l’aide de la chromatogrpahie en phase gazeuse sur colonne capillaire, Chromatographia, 5, 1972, 229-239.)NIST Spectranist ri  |
| 1090. 2 (Program type: Isothermal; Col… (show more)umn class: Standard polar; 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 cyclenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(1), 1972, 39-47., Program type: Isothermal; Col… (show more)umn class: Standard 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 Normal-Alkenen, Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatographie. Identification des alcenes, cyclopentenes et -hexenes a l’aide de la chromatogrpahie en phase gazeuse sur colonne capillaire, Chromatographia, 5, 1972, 229-239.)NIST Spectranist ri  |
| 1099. 6 (Program type: Isothermal; Col… (show more)umn class: Standard 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 cyclenes on capillary columns, Izv. Akad. Nauk Est. SSR, Khim. Geol., 21(1), 1972, 39-47., Program type: Isothermal; Col… (show more)umn class: Standard 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 Normal-Alkenen, Cyclopentenen und -Hexenen mittels Kapillar-Gas-Chromatographie. Identification des alcenes, cyclopentenes et -hexenes a l’aide de la chromatogrpahie en phase gazeuse sur colonne capillaire, Chromatographia, 5, 1972, 229-239.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

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| --- |
| 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, 1091-1097, 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; Heat rate: 3 K/min; Start T: 50 C; End T: 220 C; CAS no: 2539755; Active phase: OV-101; Carrier gas: N2; Data type: Normal alkane RI; Authors: Chupalov, A. A.; Zenkevich, I. G., Chromatographic Characterization of Structural Transformations of Organic Compounds in Diels-Alder Reaction. Aliphatic Dienes and Dienophyls, 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; Heat rate: 4 K/min; Start T: 40 C; End T: 250 C; CAS no: 2539755; Active phase: SP-2100; Carrier gas: He; Data type: Normal alkane RI; Authors: Alencar, J. W.; 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, 2008, 24-36.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 0. 8±0. 1 g/cm 3  |
| 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 3  |
| #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 2  |
| Polarizability:  | 16. 3±0. 5 10 -24 cm 3  |
| Surface Tension:  | 26. 6±3. 0 dyne/cm  |
| Molar Volume:  | 151. 8±3. 0 cm 3  |

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. 49Boiling 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. 114log Kow used: 4. 49 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 11. 045 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 83E-001 atm-m3/moleGroup Method: 1. 81E-001 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 315E-001 atm-m3/moleLog 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. 616Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6884Biowin2 (Non-Linear Model) : 0. 7764Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 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/molecule-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/molecule-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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