

# [Diisopropyl ether c6h14o structure](https://assignbuster.com/diisopropyl-ether-c6h14o-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 6 H 14 O |
| Average mass | 102. 175 Da |
| Density | 0. 8±0. 1 g/cm 3 |
| Boiling Point | 68. 3±0. 0 °C at 760 mmHg |
| Flash Point | -12. 8±0. 0 °C |
| Molar Refractivity | 31. 5±0. 3 cm 3 |
| Polarizability | 12. 5±0. 5 10 -24 cm 3 |
| Surface Tension | 20. 1±3. 0 dyne/cm |
| Molar Volume | 134. 7±3. 0 cm 3 |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Predicted – Mcule
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| -86 °CJean-Claude Bradley Open Melting Point Dataset13355 |
| -86. 8 °CJean-Claude Bradley Open Melting Point Dataset20515 |
| 0. 725 °CLabNetworkLN00163172 |

## Experimental Boiling Point:

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| --- |
| 154 F (67. 7778 °C)NIOSHTZ5425000 |
| 68 °CLabNetworkLN00163172 |

## Experimental Ionization Potent:

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| --- |
| 9. 2 EvNIOSHTZ5425000 |

## Experimental Vapor Pressure:

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| --- |
| 119 mmHgNIOSHTZ5425000 |

## Experimental Flash Point:

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| --- |
| -18 F (-27. 7778 °C)NIOSHTZ5425000 |
| -28-18 °CLabNetworkLN00163172 |

## Experimental Freezing Point:

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| --- |
| -76 F (-60 °C)NIOSHTZ5425000 |

## Experimental Gravity:

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| --- |
| 20 g/mLMerck Millipore1176, 4456 |
| 20 g/lMerck Millipore1176, 4456, 845123, 800866 |

## Experimental Refraction Index:

|  |
| --- |
| 1. 3684Alfa AesarL13215 |

## Experimental Solubility:

|  |
| --- |
| 0. 2%NIOSHTZ5425000 |
| -1. 10Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s |

* Miscellaneous

## Appearance:

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| --- |
| Colorless liquid with a sharp, sweet, ether-like odor. NIOSHTZ5425000 |

## Safety:

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| DANGER: FLAMMABLE, causes CNS effects, irritates skin & eyesAlfa AesarL13215 |

## First-Aid:

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| Eye: Irrigate immediately Skin: Soap wash promptly Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHTZ5425000 |

## Exposure Routes:

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| inhalation, ingestion, skin and/or eye contactNIOSHTZ5425000 |

## Symptoms:

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| Irritation eyes, skin, nose; respiratory discomfort; dermatitis; in animals: drowsiness, dizziness, unconsciousness, narcosisNIOSHTZ5425000 |

## Target Organs:

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| --- |
| Eyes, skin, respiratory system, central nervous systemNIOSHTZ5425000 |

## Incompatibility:

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| Strong oxidizers, acids [Note: Unstable peroxides may form on long contact with air.]NIOSHTZ5425000 |

## Personal Protection:

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| Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet (flammable) Change: No recommendationNIOSHTZ5425000 |

## Exposure Limits:

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| NIOSH REL : TWA 500 ppm (2100 mg/m 3 ) OSHA PEL : TWA 500 ppm (2100 mg/m 3 )NIOSHTZ5425000 |

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 602 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 2 mm; Column length: 100 m; Column type: Capillary; Description: 5C(10min)=> 5C/min=> 50C(48min)=> 1. 5C/min=> 195C(91min); CAS no: 108203; Active phase: Petrocol DH-100; Carrier gas: He; Data type: Kovats RI; Authors: Haagen-Smit Laboratory, Procedure for the detailed hydrocarbon analysis of gasolines by single column high efficiency (capillary) column gas chromatography, SOP NO. MLD 118, Revision No. 1. 1, California Environmental Protection Agency, Air Resources Board, El Monte, California, 1997, 22.)NIST Spectranist ri |
| 593 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 120 C; CAS no: 108203; Active phase: SE-30; Carrier gas: N2; Substrate: Supelcoport; Data type: Kovats RI; Authors: Garcia-Raso, A.; Martinez-Castro, I.; Paez, M. I.; Sanz, J.; Garcia-Raso, J.; Saura-Calixto, F., Gas Chromatographic Behaviour of Carbohydrate Trimethylsilyl Ethers. I. Aldopentoses, J. Chromatogr., 398, 1987, 9-20.)NIST Spectranist ri |
| 590 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 108203; Active phase: SE-30; Carrier gas: Ar; Substrate: Gas Chrom Q (80-100 mesh); Data type: Kovats RI; Authors: Tiess, D., Gaschromatographische Retentionsindices von 125 leicht- bis mittelfluchtigen organischen Substanzen toxikologisch-analytischer Relevanz auf SE-30, Wiss. Z. Wilhelm-Pieck-Univ. Rostock Math. Naturwiss. Reihe, 33, 1984, 6-9.)NIST Spectranist ri |
| 594 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 100 C; CAS no: 108203; Active phase: SE-30; Substrate: Gaschrom Q; Data type: Kovats RI; Authors: Winskowski, J., Gaschromatographische Identifizierung von Stoffen anhand von Indexziffem und unterschiedlichen Detektoren, Chromatographia, 17(3), 1983, 160-165.)NIST Spectranist ri |
| 624 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 200 C; CAS no: 108203; Active phase: Porapack Q; Carrier gas: N2; Data type: Kovats RI; Authors: Goebel, K.-J., Gaschromatographische Identifizierung Niedrig Siedender Substanzen Mittels Retentionsindices und Rechnerhilfe, J. Chromatogr., 235, 1982, 119-127.)NIST Spectranist ri |
| 563 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 120 C; CAS no: 108203; Active phase: Apiezon L; Substrate: Celite 545; 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 |
| 564 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 160 C; CAS no: 108203; Active phase: Apiezon L; Substrate: Celite 545; 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 |
| 570 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 25 m; Column type: Packed; Start T: 70 C; CAS no: 108203; Active phase: Apiezon L; Substrate: Celite; Data type: Kovats RI; Authors: Wehrli, A.; Kovats, E., Gas-chromatographische Charakterisierung ogranischer Verbindungen. Teil 3: Berechnung der Retentionsindices aliphatischer, alicyclischer und aromatischer Verbindungen, Helv. Chim. Acta, 7, 1959, 2709-2736., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 70 C; CAS no: 108203; Active phase: Apiezon L; 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 |
| 565 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 1 m; Column type: Packed; Start T: 130 C; CAS no: 108203; Active phase: Apiezon M; Carrier gas: N2; Substrate: Chromosorb W; Data type: Kovats RI; Authors: Golovnya, R. V.; Garbuzov, V. G., Effect of heteroatom in aliphatic sulfur- and oxygen-containing compounds on the values of the retention indices in gas chromatography, Izv. Akad. Nauk SSSR Ser. Khim., 7, 1974, 1519-1521, In original 1599-1601.)NIST Spectramainlib\_229501, replib\_19939, replib\_19940, nist ri |
| 568 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 25 m; Column type: Packed; Start T: 130 C; CAS no: 108203; Active phase: Apiezon L; Substrate: Celite; Data type: Kovats RI; Authors: Wehrli, A.; Kovats, E., Gas-chromatographische Charakterisierung ogranischer Verbindungen. Teil 3: Berechnung der Retentionsindices aliphatischer, alicyclischer und aromatischer Verbindungen, Helv. Chim. Acta, 7, 1959, 2709-2736.)NIST Spectranist ri |
| 652 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 120 C; CAS no: 108203; Active phase: Carbowax 20M; Carrier gas: N2; Substrate: Supelcoport; Data type: Kovats RI; Authors: Garcia-Raso, A.; Martinez-Castro, I.; Paez, M. I.; Sanz, J.; Garcia-Raso, J.; Saura-Calixto, F., Gas Chromatographic Behaviour of Carbohydrate Trimethylsilyl Ethers. I. Aldopentoses, J. Chromatogr., 398, 1987, 9-20.)NIST Spectranist ri |
| 679 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 2 m; Column type: Packed; Start T: 75 C; CAS no: 108203; Active phase: Carbowax 20M; Carrier gas: N2; Substrate: Kieselgur (60-100 mesh); Data type: Kovats RI; Authors: Goebel, K.-J., Gaschromatographische Identifizierung Niedrig Siedender Substanzen Mittels Retentionsindices und Rechnerhilfe, J. Chromatogr., 235, 1982, 119-127.)NIST Spectranist ri |
| 667 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 108203; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri |
| 670 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 108203; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri |
| 682 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 120 C; CAS no: 108203; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

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| --- |
| 590 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 108203; Active phase: SE-30; Data type: Normal alkane RI; Authors: Vinogradov, B. A., Production, composition, properties and application of essential oils, 2004.)NIST Spectranist ri |
| 598. 8 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 40 C; End T: 260 C; Start time: 5 min; CAS no: 108203; Active phase: DB-1; Carrier gas: He; Phase thickness: 3 um; Data type: Normal alkane RI; Authors: J&W Scientific, Solvent Retention Data, 2003.)NIST Spectranist ri |
| 568 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 108203; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Du, X., Quantitative structure-property relationship study on analysis of retention index of organic compound in gas chromatography, Chemical World (Chinese), 42(8), 2001, 403-406.)NIST Spectranist ri |
| 599. 8 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Description: 35C(4min) => 4C/min => 130C => 25C/min => 200C(5min); CAS no: 108203; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 1. 2 um; Data type: Normal alkane RI; Authors: Miermans, C. J. H.; van der Velde, L. E.; Frintrop, P. C. M., Analysis of volatile organic compounds, using the purge and trap injector coupled to a gas chromatograph/ion-trap mass spectrometer: Review of the results in Dutch surface water of the Rhine, Meuse, Northern Delta Area and Westerscheldt, over the period 1992-1997, Chemosphere, 40, 2000, 39-48.)NIST Spectranist ri |
| 600. 6 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 53 mm; Column type: Capillary; Heat rate: 4 K/min; Start T: 35 C; End T: 220 C; End time: 2 min; Start time: 10 min; CAS no: 108203; Active phase: RTX-1; Carrier gas: He; Phase thickness: 3 um; Data type: Normal alkane RI; Authors: Restek, Restek International, 1999 Product Guide, 1(1), 1999, 578-591, In original 578-591.)NIST Spectranist ri |
| 598 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 53 mm; Column length: 60 m; Column type: Capillary; Description: 40C(6min)=> 5C/min=> 80C=> 10C/min=> 200C; CAS no: 108203; Active phase: SPB-1; Carrier gas: He; Phase thickness: 5 um; Data type: Normal alkane RI; Authors: Flanagan, R. J.; Streete, P. J.; Ramsey, J. D., Volatile Substance Abuse, UNODC Technical Series, No 5, United Nations, Office on Drugs and Crime, Vienna International Centre, PO Box 500, A-1400 Vienna, Austria, 1997, 56.)NIST Spectranist ri |
| 596 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 108203; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Zenkevich, I. G.; Korolenko, L. I.; Khralenkova, N. B., Desorption with solvent vapor as a method of sample preparation in the sorption preconcentration of organic-compounds from the air of a working area and from industrial-waste gases, J. Appl. Chem. USSR (Engl. Transl.), 50(10), 1995, 937-944.)NIST Spectranist ri |
| 594 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 108203; Active phase: OV-1; Data type: Normal alkane RI; Authors: Ramsey, J. D.; Flanagan, R. J., Detection and Identification of Volatile Organic Compounds in Blood by Headspace Gas Chromatography as an Aid to the Diagnosis of Solvent Abuse, J. Chromatogr., 240, 1982, 423-444.)NIST Spectranist ri |
| 602. 4 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; CAS no: 108203; Active phase: RTX-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Wentworth, W. E.; Helias, N.; Zlatkis, A.; Chen, E. C. M.; Stearns, S. D., Multiple detector responses for gas chromatography peak identification, J. Chromatogr. A, 795, 1998, 319-347.)NIST Spectranist ri |
| 603 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 40 m; Column type: Capillary; Description: 30 0C (1 min) ^ 15 0C/min -> 45 0C ^ 3 0C/min -> 120 0C; CAS no: 108203; Active phase: CP Sil 8 CB; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Weller, J.-P.; Wolf, M., Massenspektroskopie und Headspace-GC, Beitr. Gerichtl. Med., 47, 1989, 525-532.)NIST Spectranist ri |
| 649 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 108203; Active phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Vinogradov, B. A., Production, composition, properties and application of essential oils, 2004.)NIST Spectranist ri |
| 662 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 108203; Active phase: Polyethylene Glycol; Data type: Normal alkane RI; Authors: Zenkevich, I. G.; Korolenko, L. I.; Khralenkova, N. B., Desorption with solvent vapor as a method of sample preparation in the sorption preconcentration of organic-compounds from the air of a working area and from industrial-waste gases, J. Appl. Chem. USSR (Engl. Transl.), 50(10), 1995, 937-944.)NIST Spectranist ri |

## Retention Index (Linear):

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| --- |
| 655. 4 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 27 mm; Column length: 62 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 90 C; CAS no: 108203; Active phase: PEG-20M; Data type: Linear RI; Authors: Wang, T.; Sun, Y., Correlation of Retention Indices obtained with Two Temperature Programmes, J. Chromatogr., 330, 1985, 167-171, In original 167-171.)NIST Spectranist ri |
| 657 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 27 mm; Column length: 62 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 80 C; CAS no: 108203; Active phase: PEG-20M; Data type: Linear RI; Authors: Wang, T.; Sun, Y., Correlation of Retention Indices obtained with Two Temperature Programmes, J. Chromatogr., 330, 1985, 167-171, In original 167-171.)NIST Spectranist ri |
| 658. 3 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 27 mm; Column length: 62 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 70 C; CAS no: 108203; Active phase: PEG-20M; Data type: Linear RI; Authors: Wang, T.; Sun, Y., Correlation of Retention Indices obtained with Two Temperature Programmes, J. Chromatogr., 330, 1985, 167-171, In original 167-171.)NIST Spectranist ri |
| 659 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 27 mm; Column length: 62 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 70 C; CAS no: 108203; Active phase: PEG-20M; Data type: Linear RI; Authors: Wang, T.; Sun, Y., Correlation of Retention Indices obtained with Two Temperature Programmes, J. Chromatogr., 330, 1985, 167-171, In original 167-171.)NIST Spectranist ri |

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

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| --- | --- |
| Density: | 0. 8±0. 1 g/cm 3 |
| Boiling Point: | 68. 3±0. 0 °C at 760 mmHg |
| Vapour Pressure: | 152. 3±0. 1 mmHg at 25°C |
| Enthalpy of Vaporization: | 29. 1±0. 0 kJ/mol |
| Flash Point: | -12. 8±0. 0 °C |
| Index of Refraction: | 1. 384 |
| Molar Refractivity: | 31. 5±0. 3 cm 3 |
| #H bond acceptors: | 1 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 2 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 1. 68 |
| ACD/LogD (pH 5. 5): | 1. 88 |
| ACD/BCF (pH 5. 5): | 15. 74 |
| ACD/KOC (pH 5. 5): | 250. 30 |
| ACD/LogD (pH 7. 4): | 1. 88 |
| ACD/BCF (pH 7. 4): | 15. 74 |
| ACD/KOC (pH 7. 4): | 250. 30 |
| Polar Surface Area: | 9 Å 2 |
| Polarizability: | 12. 5±0. 5 10 -24 cm 3 |
| Surface Tension: | 20. 1±3. 0 dyne/cm |
| Molar Volume: | 134. 7±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) = 1. 88Log Kow (Exper. database match) = 1. 52Exper. Ref: Funasaki, N et al. (1985)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 67. 34 (Adapted Stein & Brown method)Melting Pt (deg C): -98. 95 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 151 (Mean VP of Antoine & Grain methods)MP (exp database): -86. 8 deg CBP (exp database): 68. 5 deg CVP (exp database): 1. 49E+02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 5800log Kow used: 1. 52 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 8800 mg/L (20 deg C)Exper. Ref: HEITMANN, W ET AL (1987)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 15525 mg/LWat Sol (Exper. database match) = 8800. 00Exper. Ref: HEITMANN, W ET AL (1987)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 68E-003 atm-m3/moleGroup Method: 4. 99E-003 atm-m3/moleExper Database: 2. 28E-03 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 3. 500E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 52 (exp database)Log Kaw used: -1. 031 (exp database)Log Koa (KOAWIN v1. 10 estimate): 2. 551Log Koa (experimental database): 2. 660Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 3515Biowin2 (Non-Linear Model) : 0. 1334Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9647 (weeks )Biowin4 (Primary Survey Model) : 3. 6906 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3099Biowin6 (MITI Non-Linear Model): 0. 3423Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 0712Ready 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): 1. 99E+004 Pa (149 mm Hg)Log Koa (Exp database): 2. 660Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 51E-010 Octanol/air (Koa) model: 1. 12E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 5. 45E-009 Mackay model : 1. 21E-008 Octanol/air (Koa) model: 8. 98E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 24. 3371 E-12 cm3/molecule-secHalf-Life = 0. 439 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 5. 274 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 8. 77E-009 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 10. 5Log Koc: 1. 021 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 = 0. 470 (BCF = 2. 954)log Kow used: 1. 52 (expkow database)Volatilization from Water: Henry LC: 0. 00228 atm-m3/mole (Henry experimental database)Half-Life from Model River: 1. 291 hoursHalf-Life from Model Lake : 98. 84 hours (4. 118 days)Removal In Wastewater Treatment: Total removal: 48. 59 percentTotal biodegradation: 0. 06 percentTotal sludge adsorption: 1. 14 percentTotal to Air: 47. 40 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 19. 4 25. 2 1000 Water 61 360 1000 Soil 19. 5 720 1000 Sediment 0. 147 3. 24e+003 0 Persistence Time: 108 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop