

# [Furan c4h4o structure](https://assignbuster.com/furan-c4h4o-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 4 H 4 O  |
| Average mass  | 68. 074 Da  |
| Density  | 0. 9±0. 1 g/cm 3  |
| Boiling Point  | 31. 4±9. 0 °C at 760 mmHg  |
| Flash Point  | -35. 6±0. 0 °C  |
| Molar Refractivity  | 18. 6±0. 3 cm 3  |
| Polarizability  | 7. 4±0. 5 10 -24 cm 3  |
| Surface Tension  | 24. 8±3. 0 dyne/cm  |
| Molar Volume  | 72. 2±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -86 °CAlfa Aesar  |
| -85. 6 °COxford University Chemical Safety Data (No longer updated)More details  |
| -85. 6 °CJean-Claude Bradley Open Melting Point Dataset15814, 20453  |
| -85 °CJean-Claude Bradley Open Melting Point Dataset7253  |
| -86 °CAlfa AesarA13102  |

## Experimental Boiling Point:

|  |
| --- |
| 32-33 °CAlfa Aesar  |
| 31. 4 °COxford University Chemical Safety Data (No longer updated)More details  |
| 32-33 °CAlfa AesarA13102  |

## Experimental LogP:

|  |
| --- |
| 1. 34Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s  |

## Experimental Flash Point:

|  |
| --- |
| -35 °CAlfa Aesar  |
| -35 °COxford University Chemical Safety Data (No longer updated)More details  |
| -35 °CAlfa Aesar  |
| -35 °F (-37. 2222 °C)Alfa AesarA13102  |
| -35 °CLabNetworkLN00195280  |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLMerck Millipore3458  |
| 20 g/lMerck Millipore3458, 820594  |
| 0. 936 g/mLAlfa AesarA13102  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 42Alfa AesarA13102  |

* Miscellaneous

## Appearance:

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| colourless liquidOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

|  |
| --- |
| Stable. Substances to be avoided include strong oxidising agents, acids, peroxides and oxygen. Highlyflammable; can form explosive mixtures with air. Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| IPR-RAT LD50 5 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 3Alfa AesarA13102  |
| 45-12-19-20/22-38-48/22-68-52/53Alfa AesarA13102  |
| 53-45-61Alfa AesarA13102  |
| DangerAlfa AesarA13102  |
| DANGER: FLAMMABLE, cancer risk, irritates skin, eyes, lungsAlfa AesarA13102  |
| DANGER: FLAMMABLE, irritates skin and eyesAlfa AesarA13102  |
| H224-H350-H341-H373-H302-H332-H315-H412-EUH019Alfa AesarA13102  |
| P210-P260-P261-P303+P361+P353-P405-P501aAlfa AesarA13102  |
| Safety glasses, gloves, good ventilation. Treat as apotential carcinogen. Oxford University Chemical Safety Data (No longer updated)More details  |

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 553 (estimated with error: 68)NIST Spectramainlib\_228308, replib\_19050  |
| 500 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Start T: 100 C; CAS no: 110009; Active phase: SPB-1; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Misharina, T. A.; Beletsky, I. V.; Golovnya, R. V., Chromatographic and IR characteristics of methyl-, formyl-, and acetyl-substituted furans and thiophenes, Russ. Chem. Bull. (Engl. Transl.), 43(1), 1994, 64-69, In original 70-75.)NIST Spectranist ri  |
| 498 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 100 C; CAS no: 110009; 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  |
| 485 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 6 m; Column type: Packed; Start T: 80 C; CAS no: 110009; Active phase: SE-30; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Viani, R.; Muggler-Chavan, F.; Reymond, D.; Egli, R. H., 196. Sur la composition de l’arome de cafe, Helv. Chim. Acta, 48(195-196), 1965, 1809-1815.)NIST Spectranist ri  |
| 483 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 120 C; CAS no: 110009; 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  |
| 492 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 160 C; CAS no: 110009; 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  |
| 797 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 200 C; CAS no: 110009; 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., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 190 C; Start time: 6 min; CAS no: 110009; Active phase: DB-Wax; Carrier gas: He; Data type: Kovats RI; Authors: Shimoda, M.; Shibamoto, T., Isolation and identification of headspace volatiles from brewed coffee with an on-column GC/MS method, J. Agric. Food Chem., 38(3), 1990, 802-804.)NIST Spectranist ri  |
| 786 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column length: 5. 5 m; Column type: Packed; Heat rate: 10 K/min; Start T: 70 C; End T: 175 C; Start time: 9 min; CAS no: 110009; Active phase: PEG-20M; Carrier gas: N2; Substrate: Celite; Data type: Kovats RI; Authors: Galt, A. M.; MacLeod, G., Headspace sampling of cooked beef aroma using Tenax GC, J. Agric. Food Chem., 32(1), 1984, 59-64.)NIST Spectranist ri  |
| 779 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 152 C; CAS no: 110009; 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  |
| 790 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 179 C; CAS no: 110009; 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  |
| 798 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 110009; 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  |
| 800 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 110009; 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  |
| 802 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 200 C; CAS no: 110009; 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 (Lee):

|  |
| --- |
| 131. 1 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column length: 60 m; Column type: Capillary; CAS no: 110009; Active phase: DB-5; Data type: Lee RI; Authors: Fuentes, M. J.; Font, R.; Gomez-Rico, M. F.; Martin-Gullon, I., Pyrolysis and combustion of waste lubricant oil from diesel cars: Decomposition and pollutants, J. Anal. Appl. Pyrolysis, 79, 2007, 215-226.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 500 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 110009; Active phase: OV-101; Data type: Normal alkane RI; Authors: Shibamoto, T., Retention Indices in Essential Oil Analysis, in Capillary Gas Chromatography in Essential Oil Analysis, Sandra, P.; Bicchi, C., ed(s), Hutchig Verlag, Heidelberg, New York, 1987, 259-274., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 110009; 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  |
| 494. 7 (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: 110009; 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  |
| 492 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Heat rate: 3 K/min; Start T: -30 C; CAS no: 110009; Active phase: DB-1; Phase thickness: 1 um; Data type: Normal alkane RI; Authors: Barrefors, G.; Bjorkqvist, S.; Ramnas, O.; Petersson, G., Gas chromatographic separation of volatile furans from birchwood smoke, J. Chromatogr. A, 753, 1996, 151-155.)NIST Spectranist ri  |
| 522. 8 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 40 C; End T: 240 C; CAS no: 110009; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Moldoveanu, S. C., Pyrolysis GC/MS, present and future (recent past and present needs), J. Microcolumn Sep., 13(3), 2001, 102-125.)NIST Spectranist ri  |
| 495 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 3. 2 m; Column type: Packed; Start T: 100 C; CAS no: 110009; Active phase: Apiezon L; Data type: Normal alkane RI; Authors: Kavan, I., Analysis of odorants, Sbornik Praci UVP, 26, 1973, 128-144, In original 128-144.)NIST Spectranist ri  |
| 760 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Description: 45 0C (15 min) ^ 3 0C/min -; 75 0C ^ 5 0C/min -; 180 0C (10 min); CAS no: 110009; Active phase: Supelcowax 10; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Soria, A. C.; Martinez-Castro, I.; Sanz, J., Some aspects of dynamic headspace analysis of volatile components in honey, Foog Res. International, 41, 2008, 838-848.)NIST Spectranist ri  |
| 786 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 110009; Active phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Shibamoto, T., Retention Indices in Essential Oil Analysis, in Capillary Gas Chromatography in Essential Oil Analysis, Sandra, P.; Bicchi, C., ed(s), Hutchig Verlag, Heidelberg, New York, 1987, 259-274., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 110009; 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  |
| 802. 9 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 40 C; End T: 230 C; Start time: 7 min; CAS no: 110009; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 1 um; Data type: Normal alkane RI; Authors: J; W Scientific, Solvent Retention Data, 2003.)NIST Spectranist ri  |
| 783 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 40 C; End T: 200 C; End time: 20 min; Start time: 10 min; CAS no: 110009; Active phase: CP-Wax 52CB; Carrier gas: N2; Phase thickness: 0. 20 um; Data type: Normal alkane RI; Authors: Houeto, P.; Borron, S. W.; Marliere, F.; Baud, F. J.; Levillain, P., Development of a method for measuring volatile organic compounds in the blood of fire victims using ‘ Purge and Trap’ gas chromatography, Indoor+Built Environ., 10, 2001, 62-69.)NIST Spectranist ri  |
| 800 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 35 C; End T: 200 C; Start time: 10 min; CAS no: 110009; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Girard, B.; Durance, T., Headspace volatiles of sockeye and pink salmon as affected by retort process, Food Chem. Toxicol., 65(1), 2000, 34-39.)NIST Spectranist ri  |
| 787. 8 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 02 in; Column length: 50 ft; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 175 C; CAS no: 110009; Active phase: Carbowax 20M; Carrier gas: He; Data type: Normal alkane RI; Authors: Hruza, D. E., Sr.; van Praag, M.; Heinsohn, H., Jr., Isolation and identification of the components of the tar of hickory wood smoke, J. Agric. Food Chem., 22(1), 1974, 123-126.)NIST Spectranist ri  |

## Retention Index (Linear):

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| --- |
| 500 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 50 C; End T: 200 C; CAS no: 110009; Active phase: OV-101; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Misharina, T. A.; Golovnya, R. V.; Beletsky, I. V., Sorption properties of heterocyclic compounds differing by heteroatom in capillary gas chromatography, Russ. Chem. Bull. (Engl. Transl.), 42(7), 1993, 1167-1170, In original 1224-1227.)NIST Spectranist ri  |
| 801 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 35C(8min) =; 4C/min =; 60C =; 6C/min =; 160C=; 20C/min =; 200C(1min); CAS no: 110009; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Bianchi, F.; Careri, M.; Mangia, A.; Musci, M., Retention indices in the analysis of food aroma volatile compounds in temperature-programmed gas chromatography: Database creation and evaluation of precision and robustness, J. Sep. Sci., 39, 2007, 563-572.)NIST Spectranist ri  |
| 802 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 35C(8min) =; 4C/min =; 60C =; 6C/min =; 160C=; 20C/min =; 200C(1min); CAS no: 110009; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Bianchi, F.; Careri, M.; Mangia, A.; Musci, M., Retention indices in the analysis of food aroma volatile compounds in temperature-programmed gas chromatography: Database creation and evaluation of precision and robustness, J. Sep. Sci., 39, 2007, 563-572., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 20 C; End T: 200 C; End time: 1 min; Start time: 1 min; CAS no: 110009; Active phase: FFAP; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Ott, A.; Fay, L. B.; Chaintreau, A., Determination and origin of the aroma impact compounds of yogurt flavor, J. Agric. Food Chem., 45, 1997, 850-858.)NIST Spectranist ri  |
| 800 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column length: 3. 05 m; Column type: Packed; Heat rate: 8 K/min; Start T: 40 C; End T: 200 C; End time: 60 min; Start time: 4 min; CAS no: 110009; Active phase: Carbowax 20M; Substrate: Supelcoport; Data type: Linear RI; Authors: Peng, C. T.; Yang, Z. C.; Ding, S. F., Prediction of rentention idexes. II. Structure-retention index relationship on polar columns, J. Chromatogr., 586, 1991, 85-112.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 0. 9±0. 1 g/cm 3  |
| Boiling Point:  | 31. 4±9. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 605. 2±0. 1 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 27. 1±0. 0 kJ/mol  |
| Flash Point:  | -35. 6±0. 0 °C  |
| Index of Refraction:  | 1. 427  |
| Molar Refractivity:  | 18. 6±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 1. 38  |
| ACD/LogD (pH 5. 5):  | 1. 16  |
| ACD/BCF (pH 5. 5):  | 4. 47  |
| ACD/KOC (pH 5. 5):  | 101. 57  |
| ACD/LogD (pH 7. 4):  | 1. 16  |
| ACD/BCF (pH 7. 4):  | 4. 47  |
| ACD/KOC (pH 7. 4):  | 101. 57  |
| Polar Surface Area:  | 13 Å 2  |
| Polarizability:  | 7. 4±0. 5 10 -24 cm 3  |
| Surface Tension:  | 24. 8±3. 0 dyne/cm  |
| Molar Volume:  | 72. 2±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. 36Log Kow (Exper. database match) = 1. 34Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 59. 30 (Adapted Stein & Brown method)Melting Pt (deg C): -87. 06 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 596 (Mean VP of Antoine & Grain methods)MP (exp database): -85. 6 deg CBP (exp database): 31. 5 deg CVP (exp database): 6. 00E+02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 9751log Kow used: 1. 34 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1e+004 mg/L (25 deg C)Exper. Ref: VALVANI, SC ET AL. (1981)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 12750 mg/LWat Sol (Exper. database match) = 10000. 00Exper. Ref: VALVANI, SC ET AL. (1981)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 38E-003 atm-m3/moleGroup Method: IncompleteExper Database: 5. 40E-03 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 5. 475E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 34 (exp database)Log Kaw used: -0. 656 (exp database)Log Koa (KOAWIN v1. 10 estimate): 1. 996Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7151Biowin2 (Non-Linear Model) : 0. 8851Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0487 (weeks )Biowin4 (Primary Survey Model) : 3. 7495 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5425Biowin6 (MITI Non-Linear Model): 0. 7390Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 4544Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 8E+004 Pa (600 mm Hg)Log Koa (Koawin est ): 1. 996Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 75E-011 Octanol/air (Koa) model: 2. 43E-011 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 35E-009 Mackay model : 3E-009 Octanol/air (Koa) model: 1. 95E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 40. 5000 E-12 cm3/molecule-secHalf-Life = 0. 264 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 169 HrsOzone Reaction: No Ozone Reaction EstimationReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 2. 18E-009 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 89. 71Log Koc: 1. 953 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. 332 (BCF = 2. 147)log Kow used: 1. 34 (expkow database)Volatilization from Water: Henry LC: 0. 0054 atm-m3/mole (Henry experimental database)Half-Life from Model River: 0. 9314 hours (55. 89 min)Half-Life from Model Lake : 79. 35 hours (3. 306 days)Removal In Wastewater Treatment: Total removal: 68. 29 percentTotal biodegradation: 0. 04 percentTotal sludge adsorption: 0. 80 percentTotal to Air: 67. 45 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 8. 23 6 1000 Water 81. 1 360 1000 Soil 10. 4 720 1000 Sediment 0. 179 3. 24e+003 0 Persistence Time: 78. 1 hr

Click to predict properties on the Chemicalize site

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* 1-Click Scaffold Hop