

# [2,4-di-t-butylphenol c14h22o structure](https://assignbuster.com/24-di-t-butylphenol-c14h22o-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 14 H 22 O |
| Average mass | 206. 324 Da |
| Density | 0. 9±0. 1 g/cm 3 |
| Boiling Point | 265. 5±9. 0 °C at 760 mmHg |
| Flash Point | 115. 0±0. 0 °C |
| Molar Refractivity | 64. 9±0. 3 cm 3 |
| Polarizability | 25. 7±0. 5 10 -24 cm 3 |
| Surface Tension | 30. 1±3. 0 dyne/cm |
| Molar Volume | 221. 2±3. 0 cm 3 |

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

## Experimental Melting Point:

|  |
| --- |
| 56 °CTCID0229 |
| 53-57 °CAlfa Aesar |
| 52-57 °COxford University Chemical Safety Data (No longer updated)More details |
| 55-59 °CMerck Millipore3381, 820422 |
| 55 °CJean-Claude Bradley Open Melting Point Dataset1554 |
| 54. 5 °CJean-Claude Bradley Open Melting Point Dataset15178 |
| 56. 5 °CJean-Claude Bradley Open Melting Point Dataset20797 |
| 53-57 °CAlfa AesarA18509 |
| 54 °CBiosynthQ-200191 |
| 56-58 °CLabNetworkLN00226610 |

## Experimental Boiling Point:

|  |
| --- |
| 265 °CAlfa Aesar |
| 265 °COxford University Chemical Safety Data (No longer updated)More details |
| 265 °CAlfa AesarA18509 |
| 265 °CLabNetworkLN00226610 |

## Experimental Flash Point:

|  |
| --- |
| 129 °CAlfa Aesar |
| 115 °COxford University Chemical Safety Data (No longer updated)More details |
| 129 °CAlfa Aesar |
| 115 °CBiosynthQ-200191 |
| 129 °F (53. 8889 °C)Alfa AesarA18509 |
| 239 °CLabNetworkLN00226610 |

## Experimental Gravity:

|  |
| --- |
| 0. 887 g/mLAlfa AesarA18509 |
| 115 g/mLBiosynthQ-200191 |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 54-59 °CJ&K Scientific244431 |
| 56 °CTCI |
| 56 °CTCID0229 |

* Miscellaneous

## Appearance:

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| --- |
| light yellow crystalsOxford University Chemical Safety Data (No longer updated)More details |
| Not AvailableNovochemy[NC-30164] |

## Stability:

|  |
| --- |
| Stable. Combustible. Incompatible with acid chlorides, oxidizing agents, acid anhydrides, copper, copper alloys, bases, brass. Oxford University Chemical Safety Data (No longer updated)More details |

## Toxicity:

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| --- |
| IPR-MUS LD50 25mg kg-1Oxford University Chemical Safety Data (No longer updated)More details |

## Safety:

|  |
| --- |
| 20/21/22Novochemy[NC-30164] |
| 20/21/36/37/39Novochemy[NC-30164] |
| 26-37Alfa AesarA18509 |
| 26-37-57-60Alfa AesarA18509 |
| 36/37/38-51/53Alfa AesarA18509 |
| 9Alfa AesarA18509 |
| GHS07; GHS09BiosynthQ-200191 |
| GHS07; GHS09Novochemy[NC-30164] |
| H315; H319; H335; H410BiosynthQ-200191 |
| H315-H319-H335-H411Alfa AesarA18509 |
| H332; H403Novochemy[NC-30164] |
| P261; P273; P305+P351+P338; P501BiosynthQ-200191 |
| P261-P280-P305+P351+P338-P304+P340-P405-P501aAlfa AesarA18509 |
| P301+P310; P337+P313Novochemy[NC-30164] |
| R22Novochemy[NC-30164] |
| Safety glasses, adequate ventilation. Oxford University Chemical Safety Data (No longer updated)More details |
| WarningAlfa AesarA18509 |
| WarningBiosynthQ-200191 |
| WarningNovochemy[NC-30164] |
| WARNING: Irritates lungs, eyes, skinAlfa AesarA18509 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1555 (estimated with error: 70)NIST Spectramainlib\_228966, replib\_22572, replib\_133233 |
| 1519 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 523 K; CAS no: 96764; Active phase: SE-30; Carrier gas: He; Substrate: N\_AW\_HMDS; Data type: Kovats RI; Authors: Verevkin, S. P.; Nesterov, O. A.; Rempel, P. D.; Synkova, N. V.; Shashkin, N. P., Chromatographic determination of the products of condensation of alkylphenols with formic aldehyde, Zh. Anal. Khim., 43, 1990, 760-761.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1494 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 150 m; Column type: Capillary; Heat rate: 1 K/min; Start T: 40 C; End T: 300 C; CAS no: 96764; Active phase: Petrocol DH; Phase thickness: 1. 0 um; Data type: Normal alkane RI; Authors: Sojak, L.; Kubinec, R.; Jurdakova, H.; Hajekova, E.; Bajus, M., GC-MS of polyethylene and polypropylene thermal cracking produxts, Petroleum & Coal, 48(1), 2006, 1-14.)NIST Spectranist ri |
| 1502 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Description: 0C (3min) => 3C/min => 50C => 5C/min => 220C (30min); CAS no: 96764; Active phase: CP-Sil5 CB MS; Phase thickness: 0. 4 um; Data type: Normal alkane RI; Authors: Tirillini, B.; Verdelli, G.; Paolocci, F.; Ciccioli, P.; Frattoni, M., The volatile organic compounds from the mycelium of Tuber borchii Vitt., Phytochemistry, 55, 2000, 983-985.)NIST Spectranist ri |
| 1519 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 40C (10min) => 3C/min => 120C => 10C/min => 250C (5min); CAS no: 96764; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Ansorena, D.; Gimeno, O.; Astiasaran, I.; Bello, J., Analysis of volatile compounds by GC-MS of a dry fermented sausage: chorizo de Pamplona, Food Res. Int., 34, 2001, 67-75., Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 50 0C (5 min) ^ 2 0C/min -> 100 0C (5 min) ^ 5 0C/min -> 300 0C; CAS no: 96764; Active phase: RTX-5 MS; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Mebazaa, R.; Mahmoudi, A.; Fouchet, M.; Dos Santos, M.; Kamissoko, F.; Nafti, A.; Ben Cheikh, R.; Rega, B.; Camel, V., Characterization of volatile compounds in Tunisian fenugreek seeds, Food Chem., 115, 2009, 1326-1336., 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: 96764; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Zhao, Y.; Li, J.; Xu, Y.; Duan, H.; Fan, W.; Zhao, G., EXtraction, preparation and identification of volatile compounds in Changyu XO brandy, Chinese J. Chromatogr., 26(2), 2008, 212-222.)NIST Spectranist ri |
| 1509 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 40 0C (2 min) ^ 5 0C/min -> 80 0C ^ 7 oC/min -> 160 0C ^ 9 0C/min -> 200 0C ^ 20 0C/min -> 280 0C (10 min); CAS no: 96764; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Zhao, Y.; Li, J.; Xu, Y.; Duan, H.; Fan, W.; Zhao, G., EXtraction, preparation and identification of volatile compounds in Changyu XO brandy, Chinese J. Chromatogr., 26(2), 2008, 212-222.)NIST Spectranist ri |
| 2312 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 50 0C ^ 2 0C/min -> 100 0C (5 min) ^ 5 0C/min -> 250 0C; CAS no: 96764; Active phase: DB-FFAP; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Mebazaa, R.; Mahmoudi, A.; Fouchet, M.; Dos Santos, M.; Kamissoko, F.; Nafti, A.; Ben Cheikh, R.; Rega, B.; Camel, V., Characterization of volatile compounds in Tunisian fenugreek seeds, Food Chem., 115, 2009, 1326-1336.)NIST Spectranist ri |
| 2330 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40 0C (4 min) ^ 3 0C/min -> 50 0C ^ 5 0C/min -> 120 0C ^ 7 0C/min -> 175 0C ^ 10 0C/min -> 230 0C (8 min); CAS no: 96764; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Yongsheng, T.; Hua, L.; Hua, W.; Li, Z., Volatile composition of young Cabernet Savignon red wine from Changli Counti (China), J. Food Composition and Analysis, 21, 2008, 689-694., Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40C(3min) => 4C/min => 160C => 7C/min => 230C (8min); CAS no: 96764; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Li, H.; Tao, Y.-S.; Wang, H.; Zhang, L., Impact odorants of Chardonnay dry white wine from Changli County (China), Eur. Food Res. Technol., , 2007.)NIST Spectranist ri |
| 2270 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 40 C; End T: 220 C; End time: 10 min; Start time: 5 min; CAS no: 96764; Active phase: RTX-Wax; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Normal alkane RI; Authors: Prososki, R. A.; Etzel, M. R.; Rankin, S. A., Solvent type affects the number, distribution, and relative quantities of volatile compounds found in sweet whey powder, J. Dairy Sci., 90, 2007, 523-531.)NIST Spectranist ri |
| 2277 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 60 0C (3 min) ^ 2 0C/min -> 220 0C ^ 3 0C/min -> 245 0C (20 min); CAS no: 96764; Active phase: DB-Wax; Carrier gas: Hydrogen; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Selli, S., Volatile constituents of orange obtained from moro oranges (Citrus Sinensis L. Osbeck), J. Food Quality, 30, 2007, 330-341.)NIST Spectranist ri |
| 2315 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Description: 40 0C (5 min) ^ 4 0C/min -> 60 0C (5 min) ^ 8 0C/min -> 250 0C (3 min); CAS no: 96764; Active phase: HP-Innowax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Viegas, M. C.; Bassoli, D. G., Utilizacao do indice de retencao linear para caracterizacao de compostos volateis em cafe soluvel utilizando GC-MS e coluna HP-Innowax, Quim. Nova, 30(8), 2007, 2031-2034.)NIST Spectranist ri |
| 2321 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; CAS no: 96764; Active phase: HP-Innowax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Viegas, M. C.; Bassoli, D. G., Utilizacao do indice de retencao linear para caracterizacao de compostos volateis em cafe soluvel utilizando GC-MS e coluna HP-Innowax, Quim. Nova, 30(8), 2007, 2031-2034.)NIST Spectranist ri |

## Retention Index (Linear):

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| 1539 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 2 m; Column type: Packed; Heat rate: 4 K/min; Start T: 80 C; End T: 250 C; CAS no: 96764; Active phase: SE-30; Substrate: GasChrom Q; Data type: Linear RI; Authors: Staniewski, J., Gas chromatographic analysis of some hydroxyoxime extractants of metals, Chem. Anal. (Warsaw), 36(2), 1991, 325-333.)NIST Spectranist ri |
| 1513 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 80 C; End T: 300 C; CAS no: 96764; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Zhao C. X.; Li, X. N.; Liang Y. Z.; Fang H. Z.; Huang L. F.; Guo F. Q., Comparative analysis of chemical components of essential oils from different samples of Rhododendron with the help of chemometrics methods, Chemom. Intell. Lab. Syst., 82, 2006, 218-228.)NIST Spectranist ri |
| 1512 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 60 C; End T: 240 C; CAS no: 96764; Active phase: DB-5; Carrier gas: H2; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Nogueira, P. C. L.; Bittrich, V.; Shepherd, G. J.; Lopes, A. V.; Marsaioli, A. J., The ecological and taxonomic importance of flower volatiles of Clusia species (Guttiferae), Phytochemistry, 56, 2001, 443-452.)NIST Spectranist ri |
| 2280 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 60 C; End T: 220 C; End time: 30 min; Start time: 5 min; CAS no: 96764; Active phase: CP-Wax 52CB; Data type: Linear RI; Authors: Mahadevan, K.; Farmer, L., Key Odor Impact Compounds in Three Yeast Extract Pastes, J. Agric. Food Chem., 54, 2006, 7242-7250.)NIST Spectranist ri |
| 2327 (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: 240 C; End time: 10 min; Start time: 5 min; CAS no: 96764; Active phase: Stabilwax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Cros, S.; Lignot, B.; Bourseau, P.; Jaouen, P.; Prost, C., Desalination of mussel cooking juices by electrodialysis: effect on the aroma profile, J. Food Eng., 69, 2005, 425-436., 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: 240 C; End time: 10 min; Start time: 5 min; CAS no: 96764; Active phase: Stabilwax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Cros, S.; Vandanjon, L.; Jaouen, P.; Bourseau, P., Processing of industrial mussel cooking juices by reverse osmosis: pollution abatement and aromas recovery, 2003.)NIST Spectranist ri |
| 2316 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 35 C; End T: 195 C; End time: 90 min; Start time: 5 min; CAS no: 96764; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Chung, H. Y.; Yung, I. K. S.; Kim, J.-S., Comparison of volatile components in dried scallops (Chlamys farreri and Patinopecten yessoensis) prepared by boiling and steaming methods, J. Agric. Food Chem., 49, 2001, 192-202., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 35 C; End T: 195 C; End time: 90 min; Start time: 5 min; CAS no: 96764; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Chung, H.-Y.; Yung, I. K. S.; Ma, W. C. J.; Kim, J.-S., Analysis of volatile components in frozen and dried scallops (Patinopecten yessoensis) by gas chromatography/mass spectrometry, Food Res. Int., 35, 2002, 43-53.)NIST Spectranist ri |
| 2317 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 35 C; End T: 195 C; End time: 90 min; Start time: 5 min; CAS no: 96764; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Chung, H. Y., Volatile components in crabmeats of Charybdis feriatus, J. Agric. Food Chem., 47, 1999, 2280-2287.)NIST Spectranist ri |
| 2321 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 230 C; End time: 60 min; CAS no: 96764; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Shiratsuchi, H.; Shimoda, M.; Imayoshi, K.; Noda, K.; Osajima, Y., Volatile flavor compounds in spray-dried skim milk powder, J. Agric. Food Chem., 42, 1994, 984-988.)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: | 265. 5±9. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±0. 6 mmHg at 25°C |
| Enthalpy of Vaporization: | 52. 4±3. 0 kJ/mol |
| Flash Point: | 115. 0±0. 0 °C |
| Index of Refraction: | 1. 499 |
| Molar Refractivity: | 64. 9±0. 3 cm 3 |
| #H bond acceptors: | 1 |
| #H bond donors: | 1 |
| #Freely Rotating Bonds: | 2 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 4. 86 |
| ACD/LogD (pH 5. 5): | 4. 72 |
| ACD/BCF (pH 5. 5): | 2279. 83 |
| ACD/KOC (pH 5. 5): | 8814. 20 |
| ACD/LogD (pH 7. 4): | 4. 72 |
| ACD/BCF (pH 7. 4): | 2279. 68 |
| ACD/KOC (pH 7. 4): | 8813. 59 |
| Polar Surface Area: | 20 Å 2 |
| Polarizability: | 25. 7±0. 5 10 -24 cm 3 |
| Surface Tension: | 30. 1±3. 0 dyne/cm |
| Molar Volume: | 221. 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) = 5. 33Log Kow (Exper. database match) = 5. 19Exper. Ref: Chem Inspect Test Inst (1992)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 281. 15 (Adapted Stein & Brown method)Melting Pt (deg C): 76. 96 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00267 (Modified Grain method)MP (exp database): 56. 5 deg CBP (exp database): 263. 5 deg CVP (exp database): 4. 77E-03 mm Hg at 25 deg CSubcooled liquid VP: 0. 00977 mm Hg (25 deg C, exp database VP )Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 5. 704log Kow used: 5. 19 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 35 mg/L (25 deg C)Exper. Ref: CHEM INSPECT TEST INST (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 32. 493 mg/LWat Sol (Exper. database match) = 35. 00Exper. Ref: CHEM INSPECT TEST INST (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: PhenolsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 3. 74E-006 atm-m3/moleGroup Method: 3. 15E-006 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 271E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 19 (exp database)Log Kaw used: -3. 816 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 9. 006Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 3973Biowin2 (Non-Linear Model) : 0. 0788Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 3753 (weeks-months)Biowin4 (Primary Survey Model) : 3. 2829 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3249Biowin6 (MITI Non-Linear Model): 0. 1588Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 5154Ready 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. 3 Pa (0. 00977 mm Hg)Log Koa (Koawin est ): 9. 006Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 3E-006 Octanol/air (Koa) model: 0. 000249 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 8. 32E-005 Mackay model : 0. 000184 Octanol/air (Koa) model: 0. 0195 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 49. 1082 E-12 cm3/molecule-secHalf-Life = 0. 218 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 2. 614 HrsOzone Reaction: No Ozone Reaction EstimationReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 0. 000134 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 393E+004Log Koc: 4. 144 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. 846 (BCF = 701. 9)log Kow used: 5. 19 (expkow database)Volatilization from Water: Henry LC: 3. 15E-006 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 268. 4 hours (11. 19 days)Half-Life from Model Lake : 3049 hours (127 days)Removal In Wastewater Treatment: Total removal: 82. 89 percentTotal biodegradation: 0. 71 percentTotal sludge adsorption: 82. 16 percentTotal to Air: 0. 02 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 151 5. 23 1000 Water 9. 94 900 1000 Soil 55. 8 1. 8e+003 1000 Sediment 34. 1 8. 1e+003 0 Persistence Time: 1. 56e+003 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop