

# [Carbaryl c12h11no2 structure](https://assignbuster.com/carbaryl-c12h11no2-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula | C 12 H 11 NO 2 |
| Average mass | 201. 221 Da |
| Density | 1. 2±0. 1 g/cm 3 |
| Boiling Point | 329. 3±15. 0 °C at 760 mmHg |
| Flash Point | 153. 0±20. 4 °C |
| Molar Refractivity | 59. 0±0. 3 cm 3 |
| Polarizability | 23. 4±0. 5 10 -24 cm 3 |
| Surface Tension | 45. 1±3. 0 dyne/cm |
| Molar Volume | 170. 0±3. 0 cm 3 |

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

## Experimental Melting Point:

|  |
| --- |
| 142 °COxford University Chemical Safety Data (No longer updated)More details |
| 145 °CJean-Claude Bradley Open Melting Point Dataset21366 |
| 142 °CJean-Claude Bradley Open Melting Point Dataset12993, 15072, 8787 |
| 144 °CBiosynthQ-200795 |
| 141-143 °CLabNetworkLN00337540 |
| 142-146 °CBIONET-Key OrganicsGS-3217 |

## Experimental Boiling Point:

|  |
| --- |
| 315 °COxford University Chemical Safety Data (No longer updated)More details |

## Experimental Flash Point:

|  |
| --- |
| 202 °COxford University Chemical Safety Data (No longer updated)More details |
| 203 °CBiosynthQ-200795 |

## Experimental Gravity:

|  |
| --- |
| 1. 232 g/mLFluorochem |
| 203 g/mLBiosynthQ-200795 |
| 1. 232 g/lFluorochem239584 |

## Experimental Solubility:

|  |
| --- |
| 0. 01%NIOSHFC5950000 |

* Miscellaneous

## Appearance:

|  |
| --- |
| colourless solidOxford University Chemical Safety Data (No longer updated)More details |
| White or gray, odorless solid. [pesticide]NIOSHFC5950000 |

## Stability:

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| --- |
| Stable. Combustible; incompatible with strongoxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details |

## Safety:

|  |
| --- |
| GHS07; GHS08; GHS09BiosynthQ-200795 |
| H302; H351; H400BiosynthQ-200795 |
| P101; P273; P281; P301+P312BiosynthQ-200795 |
| Safety glasses, gloves, adequate ventilation. Oxford University Chemical Safety Data (No longer updated)More details |
| WarningBiosynthQ-200795 |

## First-Aid:

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| --- |
| Eye: Irrigate immediately Skin: Soap wash promptly Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHFC5950000 |

## Exposure Routes:

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| --- |
| inhalation, skin absorption, ingestion, skin and/or eye contactNIOSHFC5950000 |

## Symptoms:

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| Miosis, blurred vision, tear; rhinorrhea (discharge of thin mucus), salivation; sweating; abdominal cramps, nausea, vomiting, diarrhea; tremor; cyanosis; convulsions; irritation skin; possible reproductive effectsNIOSHFC5950000 |

## Target Organs:

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| --- |
| ChE inhibitorTargetMolT0790 |
| respiratory system, central nervous system, cardiovascular system, skin, blood cholinesterase, reproductive systemNIOSHFC5950000 |

## Incompatibility:

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| --- |
| Strong oxidizers, strongly alkaline pesticidesNIOSHFC5950000 |

## Personal Protection:

|  |
| --- |
| Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet or contaminated Change: DailyNIOSHFC5950000 |

## Exposure Limits:

|  |
| --- |
| NIOSH REL : TWA 5 mg/m 3 OSHA PEL : TWA 5 mg/m 3NIOSHFC5950000 |

## Bio Activity:

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| --- |
| ChETargetMolT0790 |
| NeuroscienceTargetMolT0790 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1810 (estimated with error: 89)NIST Spectramainlib\_52624, replib\_59654, replib\_157293, replib\_215734, replib\_379930 |
| 1871 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 15 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; End T: 270 C; CAS no: 63252; Active phase: DB-1; Carrier gas: He; Data type: Kovats RI; Authors: Hall, G. L.; Whitehead, W. E.; Mourer, C. R.; Shibamoto, T., A new gas chromatographic retention index for pesticides and related compounds, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 9, 1986, 266-271.)NIST Spectranist ri |
| 1903 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 50C(1min)=> 20C/min=> 150C=> 10C/min=> 280C(4min); CAS no: 63252; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Tanabe, A.; Mitobe, H.; Kawata, K.; Sakai, M.; Yasuhara, A., New monitoring system for ninety pesticides and related compounds in river water by solid-phase extraction with determination by gas chromatography/mass spectrometry, J. AOAC Int., 83(1), 2000, 61-77.)NIST Spectranist ri |
| 1931 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Start T: 200 C; CAS no: 63252; Active phase: Ultra-2; Data type: Kovats RI; Authors: Li, L.; Guan, Y.; Zhou, L., Standard Kovats indexes of 20 pesticides and their identification in temperature-programmed capillary gas chromatography., Fenxi Huaxue, 23(1), 1995, 14-19.)NIST Spectranist ri |
| 1910 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 15 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; End T: 270 C; CAS no: 63252; Active phase: DB-5; Carrier gas: He; Data type: Kovats RI; Authors: Hall, G. L.; Whitehead, W. E.; Mourer, C. R.; Shibamoto, T., A new gas chromatographic retention index for pesticides and related compounds, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 9, 1986, 266-271.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1856 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 50C(1min) => 20C/min => 120C => 5C/min => 300C(10min); CAS no: 63252; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Shimadzu Corporation, Analysis of 124 pesticides with capillary GC-FTD and GC-ECD, 2003.)NIST Spectranist ri |
| 1859. 4 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Description: 80C(1min)=> 10C/min => 150C=> 3C/min => 220C => 40C/min => 280C; CAS no: 63252; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Ma, X.; Li, C.; Tao, C.; Liu, W.; Zheng, S., Multi-residue determination of 41 insecticides in garlic by gas chromatography and ion trap mass spectrometry using the selective ion storage technique, Rapid Commun. Mass Spectrom., 15, 2001, 15-19.)NIST Spectranist ri |
| 1863. 8 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 2 mm; Column length: 12 m; Column type: Capillary; Heat rate: 18 K/min; Start T: 60 C; End T: 265 C; Start time: 1 min; CAS no: 63252; Active phase: HP-1; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Liao, W.; Joe, T.; Cusick, W. G., Multiresidue screening method for fresh fruits and vegetables with gas chromatographic/mass spectrometric detection, J. Ass. Offic. Anal. Chem, 74(3), 1991, 554-565.)NIST Spectranist ri |
| 1903. 5 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 2 mm; Column length: 12 m; Column type: Capillary; Heat rate: 18 K/min; Start T: 60 C; End T: 265 C; Start time: 1 min; CAS no: 63252; Active phase: HP-1; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Liao, W.; Joe, T.; Cusick, W. G., Multiresidue screening method for fresh fruits and vegetables with gas chromatographic/mass spectrometric detection, J. Ass. Offic. Anal. Chem, 74(3), 1991, 554-565.)NIST Spectranist ri |
| 1859. 3 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 2 mm; Column length: 25 m; Column type: Capillary; Description: 80 0C (0. 5 min) ^ 25 0C/min -> 185 0C ^ 5 0C/min -> 225 0C (3 min); CAS no: 63252; Active phase: Methyl Silicone; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Szeto, S. Y.; Price, P. M., Persistence of pesticide residues in mineral and organic soils in the Fraser Valley of British Columbia, J. Agric. Food Chem., 39(9), 1991, 1679-1684.)NIST Spectranist ri |
| 1860. 5 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 1. 1 m; Column type: Packed; Heat rate: 8. 5 K/min; Start T: 50 C; End T: 300 C; CAS no: 63252; Active phase: OV-101; Carrier gas: N2; Substrate: Chromosorb W HP; Data type: Normal alkane RI; Authors: Saxton, W. L., Emergence temperature indices and relative retention times of pesticides and industrial chemicals determined by linear programmed temperature gas chromatography, J. Chromatogr., 393, 1987, 175-194.)NIST Spectranist ri |
| 1848. 4 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 247 mm; Column length: 15 m; Column type: Capillary; Description: 1 min at 90 C; 90-150 C at 20 deg/min; 150-250 C at 5 deg/min; hold at 250 C for elution of last component; CAS no: 63252; Active phase: SE-30; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Ripley, B. D.; Braun, H. E., Retention time data for organochlorine, organophosphorus, and organonitrogen pesticides on SE-30 capillary column and application of capillary gas chromatography to pesticide residue analysis, J. Ass. Offic. Anal. Chem, 66(5), 1983, 1084-1095.)NIST Spectranist ri |
| 1865 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 2 m; Column type: Packed; Heat rate: 2. 5 K/min; Start T: 120 C; End T: 200 C; CAS no: 63252; Active phase: SE-30; Substrate: Gas Chrom P; Data type: Normal alkane RI; Authors: Marozzi, E.; Gambaro, V.; Saligari, E.; Mariani, R.; Lodi, F., Use of the retention index in gas chromatographic studies of drugs, J. Anal. Toxicol., 6, 1982, 185-192.)NIST Spectranist ri |
| 1915 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 2 m; Column type: Packed; Heat rate: 2. 5 K/min; Start T: 120 C; End T: 200 C; CAS no: 63252; Active phase: OV-1; Substrate: Gas Chrom P; Data type: Normal alkane RI; Authors: Marozzi, E.; Gambaro, V.; Saligari, E.; Mariani, R.; Lodi, F., Use of the retention index in gas chromatographic studies of drugs, J. Anal. Toxicol., 6, 1982, 185-192.)NIST Spectranist ri |
| 1867. 8 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 6 ft; Column type: Packed; CAS no: 63252; Active phase: DC-200; Carrier gas: He; Substrate: Chromosorb W HP (80-100 mesh); Data type: Normal alkane RI; Authors: Laski, R. R.; Watts, R. R., Gas chromatography of organonitrogen pesticides, using a nitrogen-specific detection system, J. Ass. Offic. Anal. Chem, 55(2), 1973, 328-332.)NIST Spectranist ri |
| 1912 (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(1 min) ^ 25 0C/min -> 125 0C ^ 10 0C/min -> 300 0C (10 min); CAS no: 63252; Active phase: 5 % Phenyl methyl siloxane; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Department of Food Safety, Ministry of Health; Welfare, Analytical methods for residual compositional substances of agricultural chemicals, feed aadditives, and veterinary drugs in foods, 2006.)NIST Spectranist ri |
| 1874 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 80C(1min) => 10C/min => 160C (5min) => 3C/min => 240C => 25C/min => 280C(10min); CAS no: 63252; Active phase: DB-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Chu, X.-G.; Hu, X.-Z.; Yao, H.-Y., Determination of 266 pesticide residues in apple juice by matrix solid-phase dispersion and gas chromatography-mass selective detection, J. Chromatogr. A, 1063, 2005, 201-210.)NIST Spectranist ri |
| 1903 (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 (1 min) ^ 20 0C/min -> 150 0C ^ 10 0C/min -> 280 0C; CAS no: 63252; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Kawara, K.; Asada, T.; Oikawa, K.; Tanabe, A., Multiresidue determination of pesticides in sediments by ultrasonically assisted extraction and gas chromatography/mass spectrometry, J. AOAC International, 88(5), 2005, 1440-1451.)NIST Spectranist ri |
| 1923. 3 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 70C(2min) => 25C/min => 150C=> 3C/min => 200C=> 8C/min => 280C(10min); CAS no: 63252; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Wong, J. W.; Webster, M. G.; Bezabeh, D. Z.; Hengel, M. J.; Ngim, K. K.; Krynitsky, A. J.; Ebeler, S. E., Multiresidue determination of pesticides in malt beverages by capillary gas chromatography with mass spectrometry and selected ion monitoring, J. Agric. Food Chem., 52, 2004, 6361-6372.)NIST Spectranist ri |
| 1879. 5 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 50C(1min) => 20C/min => 120C => 5C/min => 300C(10min); CAS no: 63252; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Shimadzu Corporation, Analysis of 124 pesticides with capillary GC-FTD and GC-ECD, 2003.)NIST Spectranist ri |
| 1887. 6 (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 (3 min) ^ 25 0C/min -> 125 0C ^ 10 0C/min -> 275 0C (25 min); CAS no: 63252; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Lehotay, S. J., Analysis of pesticide residues in mixed fruit and vegetable extracts by direct sample introduction/gas chromatography/tandem mass spectrometry, J. AOAC Int., 83(3), 2000, 680-697.)NIST Spectranist ri |
| 1899. 3 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 70C(0. 5min) => 10C/min=> 270C(0. 1min) => 25C/min => 290C(2min); CAS no: 63252; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Soleas, G. J.; Yan, J.; Hom, K.; Goldberg, D. M., Multiresidue analysis of seventeen pesticides in wine by gas chromatography with mass-selective detection, J. Chromatogr. A, 882, 2000, 205-212.)NIST Spectranist ri |
| 1893. 1 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 25 m; Column type: Capillary; Description: 100C(1min) => 30C/min=> 150C(2min) => 3C/min=> 205C => 10C/min => 260C(29min); CAS no: 63252; Active phase: SE-54; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Stan, H.-J., Pesticide residue analysis in foodstuffs applying capillary gas chromatography with mass spectrometric detection State-of-the-art use of modified DFG-multimethod S19 and automated data evaluation, J. Chromatogr. A, 892, 2000, 347-377.)NIST Spectranist ri |
| 1888. 4 (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 C (1. 13 min) ^ 30 C/min -> 150 C ^ 3 C/min -> 205 C ^ 10 C/min -> 250 C (20 min); CAS no: 63252; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Cook, J.; Engel, M.; Wylie, P.; Quimby, B., Multiresidue screening of pesticides in foods using retention time locking, GC-AED, database search, and GC/MS identification, J. AOAC Int., 82(2), 1999, 313-326.)NIST Spectranist ri |
| 1914. 7 (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: 6 K/min; Start T: 60 C; End T: 260 C; End time: 12 min; CAS no: 63252; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Mogadati, P.; Louis, J. B.; Rosen, J. D., Multiresidue determination of pesticides in high-organic-content soils by solid-phase extraction and gas chromatography/mass spectrometry, J. AOAC Int., 82(3), 1999, 705-715.)NIST Spectranist ri |
| 1911. 8 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Description: 50 C(2min) => 20C/min => 150C => 6C/min => 280C (30min); CAS no: 63252; Active phase: NB-54; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Tamura, Y.; Nagayama, T.; Kobayashi, M.; Hiashimoto, T.; Haneishi, N.; Ito, M.; Tomomatsu, T., Simultaneous determination of organonitrogen and carbamate pescticides in foods by an internal standard method based on retention indices in dual-column gas chromatography, Shokuhin Eiseigaku Zasshi, 39(3), 1998, 225-232.)NIST Spectranist ri |
| 1875. 7 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 25 m; Column type: Capillary; Description: 85 0C (1 min) ^ 40 0C/min -> 150 0C (2 min) ^ 10 0C/min -> 280 0C (20 min); CAS no: 63252; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Holland, P. T.; McNaughton, D. E.; Malcolm, C. P., Multiresidue analysis of pesticides in wines by solid-phase extraction, J. AOAC Int., 77(1), 1994, 79-86.)NIST Spectranist ri |
| 2826 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 63252; Active phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Tameo, O.; Kiyos, I., Simultaneous determination of pesticides by capillary gas chromatography, Cannot be traslated (in Japan), 14(2), 1991, 109-122.)NIST Spectranist ri |

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

|  |  |
| --- | --- |
| Density: | 1. 2±0. 1 g/cm 3 |
| Boiling Point: | 329. 3±15. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±0. 7 mmHg at 25°C |
| Enthalpy of Vaporization: | 57. 2±3. 0 kJ/mol |
| Flash Point: | 153. 0±20. 4 °C |
| Index of Refraction: | 1. 611 |
| Molar Refractivity: | 59. 0±0. 3 cm 3 |
| #H bond acceptors: | 3 |
| #H bond donors: | 1 |
| #Freely Rotating Bonds: | 2 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 2. 40 |
| ACD/LogD (pH 5. 5): | 2. 44 |
| ACD/BCF (pH 5. 5): | 41. 95 |
| ACD/KOC (pH 5. 5): | 504. 86 |
| ACD/LogD (pH 7. 4): | 2. 44 |
| ACD/BCF (pH 7. 4): | 41. 95 |
| ACD/KOC (pH 7. 4): | 504. 85 |
| Polar Surface Area: | 38 Å 2 |
| Polarizability: | 23. 4±0. 5 10 -24 cm 3 |
| Surface Tension: | 45. 1±3. 0 dyne/cm |
| Molar Volume: | 170. 0±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) = 2. 35Log Kow (Exper. database match) = 2. 36Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 327. 50 (Adapted Stein & Brown method)Melting Pt (deg C): 91. 20 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 5. 33E-005 (Modified Grain method)MP (exp database): 145 deg CBP (exp database): 315 deg CVP (exp database): 1. 36E-06 mm Hg at 25 deg CSubcooled liquid VP: 2. 09E-005 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): 416. 2log Kow used: 2. 36 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 110 mg/L (22 deg C)Exper. Ref: PESTICIDE PROP DATABASEWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 206. 8 mg/LWat Sol (Exper. database match) = 110. 00Exper. Ref: PESTICIDE PROP DATABASEECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 3. 14E-009 atm-m3/moleGroup Method: IncompleteExper Database: 4. 36E-09 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 3. 391E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 36 (exp database)Log Kaw used: -6. 749 (exp database)Log Koa (KOAWIN v1. 10 estimate): 9. 109Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7313Biowin2 (Non-Linear Model) : 0. 7615Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7078 (weeks-months)Biowin4 (Primary Survey Model) : 3. 7510 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 1280Biowin6 (MITI Non-Linear Model): 0. 1188Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 0885Ready 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): 0. 00279 Pa (2. 09E-005 mm Hg)Log Koa (Koawin est ): 9. 109Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 00108 Octanol/air (Koa) model: 0. 000316 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0374 Mackay model : 0. 0793 Octanol/air (Koa) model: 0. 0246 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 25. 9969 E-12 cm3/molecule-secHalf-Life = 0. 411 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 4. 937 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 0584 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 241. 7Log Koc: 2. 383 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 4. 680E+000 L/mol-secKb Half-Life at pH 8: 1. 714 days Kb Half-Life at pH 7: 17. 143 days Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 1. 117 (BCF = 13. 1)log Kow used: 2. 36 (expkow database)Volatilization from Water: Henry LC: 4. 36E-009 atm-m3/mole (Henry experimental database)Half-Life from Model River: 1. 905E+005 hours (7937 days)Half-Life from Model Lake : 2. 078E+006 hours (8. 659E+004 days)Removal In Wastewater Treatment: Total removal: 2. 76 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 66 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0346 9. 87 1000 Water 18. 1 900 1000 Soil 81. 7 1. 8e+003 1000 Sediment 0. 116 8. 1e+003 0 Persistence Time: 1. 51e+003 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop