

# [Nikethamide c10h14n2o structure](https://assignbuster.com/nikethamide-c10h14n2o-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 10 H 14 N 2 O |
| Average mass | 178. 231 Da |
| Density | 1. 0±0. 1 g/cm 3 |
| Boiling Point | 298. 0±0. 0 °C at 760 mmHg |
| Flash Point | 141. 1±20. 4 °C |
| Molar Refractivity | 52. 0±0. 3 cm 3 |
| Polarizability | 20. 6±0. 5 10 -24 cm 3 |
| Surface Tension | 40. 6±3. 0 dyne/cm |
| Molar Volume | 171. 0±3. 0 cm 3 |

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

## Experimental Melting Point:

|  |
| --- |
| 24-26 °COxford University Chemical Safety Data (No longer updated)More details |
| 25 °CJean-Claude Bradley Open Melting Point Dataset15953, 21485 |

## Experimental Boiling Point:

|  |
| --- |
| 296 °COxford University Chemical Safety Data (No longer updated)More details |

## Experimental Flash Point:

|  |
| --- |
| 22 °CTCID0514 |
| 112 °COxford University Chemical Safety Data (No longer updated)More details |

* Miscellaneous

## Appearance:

|  |
| --- |
| light yellow viscous liquidOxford University Chemical Safety Data (No longer updated)More details |

## Toxicity:

|  |
| --- |
| IVN-RAT LD50 191 mg kg-1, SCU-RAT LD50 240 mg kg-1, ORL-MUS LD50 188 mg kg-1, ORL-RBT LD50 650 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details |

## Safety:

|  |
| --- |
| DangerBiosynthW-105333 |
| GHS06BiosynthW-105333 |
| H301; H315; H319; H335BiosynthW-105333 |
| P261; P301+P310; P305+P351+P338BiosynthW-105333 |
| Safety glasses. Oxford University Chemical Safety Data (No longer updated)More details |

## Target Organs:

|  |
| --- |
| GABARTargetMolT0048 |

## Bio Activity:

|  |
| --- |
| GABARTargetMolT0048 |
| NeuroscienceTargetMolT0048 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1386 (estimated with error: 83)NIST Spectramainlib\_291418, replib\_42285, replib\_234082 |
| 1520 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 140 C; CAS no: 59267; Active phase: SE-30; Carrier gas: N2; Substrate: 1% se-30 on Anachrom ABS(80-100mesh); Data type: Kovats RI; Authors: Musumarra, G.; Scarlata, G.; Romano, G.; Cappello, G.; Clementi, S.; Giulietti, G., Qualitative organic analysis. Part 2. Identification of drugs by principal components analysis of standardized TLC data in four eluent systems and of retention indices on SE 30, J. Anal. Toxicol., 11, 1987, 154-163.)NIST Spectranist ri |
| 1515 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 49 mm; Column length: 25 m; Column type: Capillary; Heat rate: 8 K/min; Start T: 100 C; End T: 275 C; End time: 15 min; Start time: 2 min; CAS no: 59267; Active phase: SE-30; Phase thickness: 1. 14 um; Data type: Kovats RI; Authors: Schepers, P.; Wijsbeek, J.; Franke, J. P.; de Zeeuw, R. A., Applicability of capillary gas chromatography to substance identification in toxicology by means of retention indices, J. Forensic Sci., 27(1), 1982, 49-60.)NIST Spectranist ri |
| 1536 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 22 mm; Column length: 12 m; Column type: Capillary; Heat rate: 8 K/min; Start T: 120 C; End T: 300 C; End time: 12 min; Start time: 2 min; CAS no: 59267; Active phase: SE-30; Carrier gas: He; Phase thickness: 0. 45 um; Data type: Kovats RI; Authors: Schepers, P.; Wijsbeek, J.; Franke, J. P.; de Zeeuw, R. A., Applicability of capillary gas chromatography to substance identification in toxicology by means of retention indices, J. Forensic Sci., 27(1), 1982, 49-60.)NIST Spectranist ri |
| 1530 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 6 ft; Column type: Packed; CAS no: 59267; Active phase: OV-101; Carrier gas: N2; Substrate: Chromosorb W; Data type: Kovats RI; Authors: McLinden, V. J.; Stenhouse, A. M., A chromatography system for drug identification, Forensic Sci. Int., 13, 1979, 71-79.)NIST Spectranist ri |
| 1503 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Packed; Start T: 150 C; CAS no: 59267; Active phase: OV-101; Substrate: Gas Chrom Q (80-100 mesh); Data type: Kovats RI; Authors: Delley, R.; Friedrich, K., System CG 72 von bevorzugten Trennflussigkeiten fur die Gas-Chromatographie, Chromatographia, 10(10), 1977, 593-600.)NIST Spectranist ri |
| 1500 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; CAS no: 59267; Active phase: SE-30; Data type: Kovats RI; Authors: Moffat, A. C.; Stead, A. H.; Smalldon, K. W., Optimum use of paper, thin-layer and gas-liquid chromatography for the identification of basic drugs. III. Gas-liquid chromatography, J. Chromatogr., 90, 1974, 19-33.)NIST Spectranist ri |
| 1487 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 160 C; CAS no: 59267; Active phase: Apiezon L; Data type: Kovats RI; Authors: Huber, J. F. K.; Kenndler, E.; Reich, G., Quantitation of the Information Content of Multi-Dimensional Gas Chromatography and Low- Resolution Mass Spectrometry in the Identification of Doping Drugs, J. Chromatogr., 172, 1979, 15-30.)NIST Spectranist ri |
| 1486 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 160 C; CAS no: 59267; Active phase: Apiezon L; Substrate: Chromosorb W; Data type: Kovats RI; Authors: Donike, M.; Stratmann, D., Gas-chromatographische identifizierung von stimulantien der phenylathylaminreihe mit hilfe der retnetions-indices, Z. Anal. Chem., 279(2), 1976, 129-131.)NIST Spectranist ri |
| 2319 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Packed; Start T: 180 C; CAS no: 59267; Active phase: PEG-20M; Carrier gas: N2; Data type: Kovats RI; Authors: Huber, J. F. K.; Kenndler, E.; Reich, G., Quantitation of the Information Content of Multi-Dimensional Gas Chromatography and Low- Resolution Mass Spectrometry in the Identification of Doping Drugs, J. Chromatogr., 172, 1979, 15-30., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Packed; Start T: 180 C; CAS no: 59267; Active phase: PEG-20M; Substrate: Chromosorb W; Data type: Kovats RI; Authors: Donike, M.; Stratmann, D., Gas-chromatographische identifizierung von stimulantien der phenylathylaminreihe mit hilfe der retnetions-indices, Z. Anal. Chem., 279(2), 1976, 129-131.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1505 (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: 59267; 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 |
| 1510 (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: 59267; 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 |
| 1525 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Other; CAS no: 59267; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.)NIST Spectranist ri |
| 1528. 7 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 12. 5 m; Column type: Capillary; Heat rate: 25 K/min; Start T: 75 C; End T: 320 C; End time: 2 min; CAS no: 59267; Active phase: Ultra-2; Phase thickness: 0. 11 um; Data type: Normal alkane RI; Authors: Hemmersbach, P.; de la Torre, R., Review. Stimulants, narcotics and . beta.-blockers: 25 years of development in analytical techniques for doping control, J. Chromatogr. B, 687, 1996, 221-238.)NIST Spectranist ri |
| 1457 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1459 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1462 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1463 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1464 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1466 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1470 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1503 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 190 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1506 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 190 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 1511 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 190 C; CAS no: 59267; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 2375 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 190 C; CAS no: 59267; Active phase: Carbowax 20M / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |
| 2386 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 190 C; CAS no: 59267; Active phase: Carbowax 20M / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri |

## Retention Index (Linear):

|  |
| --- |
| 1497 (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: 8 K/min; Start T: 120 C; End T: 280 C; End time: 5 min; CAS no: 59267; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Perrigo, B. J.; Ballantyne, D. J.; Peel, H. W., Condierations in developing a data base for drugs on a DBI capillary column, J. Can. Soc. Forensic Sci., 17(2), 1984, 41-49., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 15 m; Column type: Capillary; Heat rate: 8 K/min; Start T: 120 C; End T: 280 C; End time: 5 min; CAS no: 59267; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Perrigo, B. J.; Peel, H. W.; Ballantyne, D. J., Use of Dual-Column Fused-Silica Capillary Gas Chromatography in Combination with Detector Response Factors for Analytical Toxicology., J. Chromatogr., 341, 1985, 81-88.)NIST Spectranist ri |
| 1494 (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: 5 K/min; Start T: 120 C; End T: 280 C; End time: 5 min; CAS no: 59267; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Perrigo, B. J.; Ballantyne, D. J.; Peel, H. W., Condierations in developing a data base for drugs on a DBI capillary column, J. Can. Soc. Forensic Sci., 17(2), 1984, 41-49.)NIST Spectranist ri |
| 1500 (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: 12 K/min; Start T: 120 C; End T: 280 C; End time: 5 min; CAS no: 59267; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Perrigo, B. J.; Ballantyne, D. J.; Peel, H. W., Condierations in developing a data base for drugs on a DBI capillary column, J. Can. Soc. Forensic Sci., 17(2), 1984, 41-49., 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: 15 K/min; Start T: 120 C; End T: 280 C; End time: 5 min; CAS no: 59267; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Perrigo, B. J.; Ballantyne, D. J.; Peel, H. W., Condierations in developing a data base for drugs on a DBI capillary column, J. Can. Soc. Forensic Sci., 17(2), 1984, 41-49., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 1. 8 m; Column type: Packed; Heat rate: 8 K/min; Start T: 130 C; End T: 290 C; End time: 8 min; Start time: 2 min; CAS no: 59267; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb W; Data type: Linear RI; Authors: Perrigo, B. J.; Peel, H. W., The use of retention indices and temperature-programmed gas chromatography in analytical toxicology, J. Chromatogr. Sci., 19, 1981, 219-226.)NIST Spectranist ri |

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

|  |  |
| --- | --- |
| Density: | 1. 0±0. 1 g/cm 3 |
| Boiling Point: | 298. 0±0. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±0. 6 mmHg at 25°C |
| Enthalpy of Vaporization: | 53. 8±3. 0 kJ/mol |
| Flash Point: | 141. 1±20. 4 °C |
| Index of Refraction: | 1. 520 |
| Molar Refractivity: | 52. 0±0. 3 cm 3 |
| #H bond acceptors: | 3 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 3 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 0. 33 |
| ACD/LogD (pH 5. 5): | 0. 54 |
| ACD/BCF (pH 5. 5): | 1. 51 |
| ACD/KOC (pH 5. 5): | 46. 52 |
| ACD/LogD (pH 7. 4): | 0. 54 |
| ACD/BCF (pH 7. 4): | 1. 52 |
| ACD/KOC (pH 7. 4): | 47. 06 |
| Polar Surface Area: | 33 Å 2 |
| Polarizability: | 20. 6±0. 5 10 -24 cm 3 |
| Surface Tension: | 40. 6±3. 0 dyne/cm |
| Molar Volume: | 171. 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) = 0. 52Log Kow (Exper. database match) = 0. 33Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 300. 45 (Adapted Stein & Brown method)Melting Pt (deg C): 88. 39 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00217 (Modified Grain method)MP (exp database): 25 deg CBP (exp database): 298 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1438log Kow used: 0. 33 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1e+006 mg/L (25 deg C)Exper. Ref: MERCK (1989)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 98958 mg/LWat Sol (Exper. database match) = 1000000. 00Exper. Ref: MERCK (1989)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 46E-011 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 539E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 33 (exp database)Log Kaw used: -8. 998 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 9. 328Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7183Biowin2 (Non-Linear Model) : 0. 8221Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5369 (weeks-months)Biowin4 (Primary Survey Model) : 3. 7773 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4076Biowin6 (MITI Non-Linear Model): 0. 3067Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 4204Ready 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. 289 Pa (0. 00217 mm Hg)Log Koa (Koawin est ): 9. 328Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 04E-005 Octanol/air (Koa) model: 0. 000522 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000374 Mackay model : 0. 000829 Octanol/air (Koa) model: 0. 0401 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 23. 3306 E-12 cm3/molecule-secHalf-Life = 0. 458 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 5. 501 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000602 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 331. 3Log Koc: 2. 520 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. 500 (BCF = 3. 162)log Kow used: 0. 33 (expkow database)Volatilization from Water: Henry LC: 2. 46E-011 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 3. 177E+007 hours (1. 324E+006 days)Half-Life from Model Lake : 3. 466E+008 hours (1. 444E+007 days)Removal In Wastewater Treatment: Total removal: 1. 86 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 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. 000338 11 1000 Water 45 900 1000 Soil 54. 9 1. 8e+003 1000 Sediment 0. 0883 8. 1e+003 0 Persistence Time: 991 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop