

# [3-vinyltoluene c9h10 structure](https://assignbuster.com/3-vinyltoluene-c9h10-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 9 H 10  |
| Average mass  | 118. 176 Da  |
| Density  | 0. 9±0. 1 g/cm 3  |
| Boiling Point  | 170. 0±10. 0 °C at 760 mmHg  |
| Flash Point  | 51. 1±0. 0 °C  |
| Molar Refractivity  | 42. 0±0. 3 cm 3  |
| Polarizability  | 16. 7±0. 5 10 -24 cm 3  |
| Surface Tension  | 30. 7±3. 0 dyne/cm  |
| Molar Volume  | 131. 7±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -82–81 °CAlfa Aesar  |
| -86 °CJean-Claude Bradley Open Melting Point Dataset13501  |
| -86. 3 °CJean-Claude Bradley Open Melting Point Dataset20683  |
| -82 °CJean-Claude Bradley Open Melting Point Dataset4121  |
| -82–81 °CAlfa AesarL08072  |

## Experimental Boiling Point:

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| --- |
| 170-171 °CAlfa Aesar  |
| 170-171 °CAlfa AesarL08072  |

## Experimental Flash Point:

|  |
| --- |
| 51 °CAlfa Aesar  |
| 51 °CAlfa Aesar  |
| 51 °F (10. 5556 °C)Alfa AesarL08072  |
| 60 °CLabNetworkLN00238850  |

## Experimental Gravity:

|  |
| --- |
| 0. 9 g/mLAlfa AesarL08072  |

## Experimental Refraction Index:

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| --- |
| 1. 541Alfa AesarL08072  |

* Miscellaneous

## Safety:

|  |
| --- |
| 10-36/37/38-65Alfa AesarL08072  |
| 26-37-62Alfa AesarL08072  |
| 3Alfa AesarL08072  |
| DangerAlfa AesarL08072  |
| DANGER: FLAMMABLE, irritates skin and eyesAlfa AesarL08072  |
| H304-H226-H315-H319-H335Alfa AesarL08072  |
| HARMFUL / IRRITANTAlfa AesarL08072  |
| P210-P301+P310-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarL08072  |

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 996 (estimated with error: 55)NIST Spectramainlib\_2023, replib\_118474, replib\_231965  |
| 956 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 0 C; CAS no: 100801; Active phase: OV-101; Data type: Kovats RI; Authors: Skrbic, B. D.; Vojinovic-Miloradov, M. B., A contribution to the qualitative GC analysis of some non-chlorinated xenobiotic chemicals in waste waters, Water Sci. Technol., 30(3), 1994, 91-93.)NIST Spectranist ri  |
| 977 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 100 m; Column type: Capillary; Start T: 96 C; CAS no: 100801; Active phase: Squalane; Carrier gas: He; Data type: Kovats RI; Authors: Kugucheva, E. E.; Mashinsky, V. I., Retention Indices of Aromatic Hydrocarbons on Capillary Columns with Squalan and Polyphenyl Ether, Zh. Anal. Khim. (Rus), 38(11), 1983, 2023-2026., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 15 m; Column type: Capillary; Start T: 70 C; CAS no: 100801; Active phase: SE-30; Carrier gas: N2; Data type: Kovats RI; Authors: Toth, T., Use of capillary gas chromatography in collecting retention and chemical information for the analysis of complex petrochemical mixtures, J. Chromatogr., 279, 1983, 157-165.)NIST Spectranist ri  |
| 960. 5 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 15 m; Column type: Capillary; Start T: 70 C; CAS no: 100801; Active phase: SE-30; Carrier gas: N2; Data type: Kovats RI; Authors: Toth, T., Use of capillary gas chromatography in collecting retention and chemical information for the analysis of complex petrochemical mixtures, J. Chromatogr., 279, 1983, 157-165.)NIST Spectranist ri  |
| 1000 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 5 mm; Column length: 100 m; Column type: Capillary; Start T: 130 C; CAS no: 100801; Active phase: SE-30; Data type: Kovats RI; Authors: Bredael, P., Retention indices of hydrocarbons on SE-30, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 5, 1982, 325-328.)NIST Spectranist ri  |
| 982 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 5 mm; Column length: 100 m; Column type: Capillary; Start T: 80 C; CAS no: 100801; Active phase: SE-30; Data type: Kovats RI; Authors: Bredael, P., Retention indices of hydrocarbons on SE-30, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 5, 1982, 325-328.)NIST Spectranist ri  |
| 985. 9 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 3 mm; Column length: 50 m; Column type: Capillary; Start T: 100 C; CAS no: 100801; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Gerasimenko, V. A.; Kirilenko, A. V.; Nabivach, V. M., Capillary gas chromatography of aromatic compounds found in coal tar fractions, J. Chromatogr., 208, 1981, 9-16.)NIST Spectranist ri  |
| 991. 4 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 3 mm; Column length: 50 m; Column type: Capillary; Start T: 120 C; CAS no: 100801; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Gerasimenko, V. A.; Kirilenko, A. V.; Nabivach, V. M., Capillary gas chromatography of aromatic compounds found in coal tar fractions, J. Chromatogr., 208, 1981, 9-16.)NIST Spectranist ri  |
| 997. 8 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 3 mm; Column length: 50 m; Column type: Capillary; Start T: 140 C; CAS no: 100801; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Gerasimenko, V. A.; Kirilenko, A. V.; Nabivach, V. M., Capillary gas chromatography of aromatic compounds found in coal tar fractions, J. Chromatogr., 208, 1981, 9-16.)NIST Spectranist ri  |
| 972. 7 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 5 mm; Column length: 25. 5 m; Column type: Capillary; Start T: 65 C; CAS no: 100801; Active phase: SE-30; Carrier gas: He; Data type: Kovats RI; Authors: Svob, V.; Deur-Siftar, D.; Cramers, C. A., Mechanisms of the thermal degradation of alkylbenzenes, J. Chromatogr., 91, 1974, 659-675.)NIST Spectranist ri  |
| 973. 2 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 5 mm; Column length: 25. 5 m; Column type: Capillary; Start T: 65 C; CAS no: 100801; Active phase: SE-30; Carrier gas: He; Data type: Kovats RI; Authors: Svob, V.; Deur-Siftar, D., Kovats Retention Indices in the Identification of Alkylbenzene Degradation Products, J. Chromatogr., 91, 1974, 677-689., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 5 mm; Column length: 25. 5 m; Column type: Capillary; Start T: 65 C; CAS no: 100801; Active phase: SE-30; Carrier gas: He; Data type: Kovats RI; Authors: Svob, V.; Deur-Siftar, D.; Cramers, C. A., Mechanisms of the thermal degradation of alkylbenzenes, J. Chromatogr., 91, 1974, 659-675.)NIST Spectranist ri  |
| 980 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 100 m; Column type: Capillary; Start T: 106 C; CAS no: 100801; Active phase: Squalane; Carrier gas: He; Data type: Kovats RI; Authors: Kugucheva, E. E.; Mashinsky, V. I., Retention Indices of Aromatic Hydrocarbons on Capillary Columns with Squalan and Polyphenyl Ether, Zh. Anal. Khim. (Rus), 38(11), 1983, 2023-2026.)NIST Spectranist ri  |
| 976. 3 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 86 C; CAS no: 100801; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Macak, J.; Nabivach, V.; Buryan, P.; Sindler, S., Dependence of retention indices of alkylbenzenes on their molecular structure, J. Chromatogr., 234, 1982, 285-302., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 86 C; CAS no: 100801; Active phase: Squalane; Data type: Kovats RI; Authors: Nabivach, V. M.; Bur’yan, P.; Matsak, I., Retention indices of aromatic hydrocarbons on a squalane capillary column, Zh. Anal. Khim., 33(7), 1978, 1108-1113, In original 1416-1422.)NIST Spectranist ri  |
| 978. 7 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 96 C; CAS no: 100801; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Macak, J.; Nabivach, V.; Buryan, P.; Sindler, S., Dependence of retention indices of alkylbenzenes on their molecular structure, J. Chromatogr., 234, 1982, 285-302., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 96 C; CAS no: 100801; Active phase: Squalane; Data type: Kovats RI; Authors: Nabivach, V. M.; Bur’yan, P.; Matsak, I., Retention indices of aromatic hydrocarbons on a squalane capillary column, Zh. Anal. Khim., 33(7), 1978, 1108-1113, In original 1416-1422.)NIST Spectranist ri  |
| 1385. 2 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Start T: 110 C; CAS no: 100801; Active phase: Carbowax 20M; Carrier gas: N2; Phase thickness: 0. 3 um; Data type: Kovats RI; Authors: Boneva, S.; Vassilev, K., Gas chromatographic separation of epoxystyrenes on carbowax 20 M capillary column, Chromatographia, 43(3/4), 1996, 208-210.)NIST Spectranist ri  |
| 1396. 8 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Start T: 120 C; CAS no: 100801; Active phase: Carbowax 20M; Carrier gas: N2; Phase thickness: 0. 3 um; Data type: Kovats RI; Authors: Boneva, S.; Vassilev, K., Gas chromatographic separation of epoxystyrenes on carbowax 20 M capillary column, Chromatographia, 43(3/4), 1996, 208-210.)NIST Spectranist ri  |
| 1348. 1 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 3 mm; Column length: 30 m; Column type: Capillary; Start T: 70 C; CAS no: 100801; Active phase: PEG-20M; Carrier gas: N2; Data type: Kovats RI; Authors: Toth, T., Use of capillary gas chromatography in collecting retention and chemical information for the analysis of complex petrochemical mixtures, J. Chromatogr., 279, 1983, 157-165.)NIST Spectranist ri  |
| 1388. 1 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Packed; Start T: 150 C; CAS no: 100801; Active phase: Carbowax 20M; Substrate: Chromosorb W, AW-DMCS; Data type: Kovats RI; Authors: Ellis, T. S.; Still, R. H., Thermal degradation of polymers. XXI. Vacuum pyrolysis of poly(m-N, N-dimethylaminostyrene); the products volatile at pyrolysis temperature, liquid at room temperature, J. Appl. Polym. Sci., 23, 1979, 2837-2854.)NIST Spectranist ri  |
| 1387. 4 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Packed; Start T: 150 C; CAS no: 100801; Active phase: Carbowax 20M; Substrate: Chromosorb W, AW-DMCS; Data type: Kovats RI; Authors: Ellis, T. S.; Still, R. H., Thermal degradation of polymers. XXI. Vacuum pyrolysis of poly(m-N, N-dimethylaminostyrene); the products volatile at pyrolysis temperature, liquid at room temperature, J. Appl. Polym. Sci., 23, 1979, 2837-2854.)NIST Spectranist ri  |

## Retention Index (Lee):

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| --- |
| 156. 2 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; CAS no: 100801; Active phase: DB-5MS; Data type: Lee RI; Authors: Aracil, I.; Font, R.; Conesa, J. A., Semivolatile and volatile compounds from the pyrolysis and combustion of polyvinyl chloride, J. Anal. Appl. Pyrolysis, 74, 2005, 465-478.)NIST Spectranist ri  |
| 158. 1 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 280 C; End time: 30 min; CAS no: 100801; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Lee RI; Authors: Wang, S.-F.; Liu, B.-Z.; Sun, K.-J.; Su, Q.-D., Gas chromatographic-mass spectrometric determination of polycyclic aromatic hydrocarbons formed during the pyrolysis of phenylalanine, J. Chromatogr. A, 1025, 2004, 255-261.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

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| --- |
| 960 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 100801; Active phase: Polymethylsiloxane, (PMS-20000); Data type: Normal alkane RI; Authors: Cornwell, E.; Cordano, G., Nueva proposicion para predecir datos de retencion obtenidos mediante cromatografia de gases de hidrocarburos derivados de las naftas, Revista de la Sociedad Quimica de Mexico, 47(1), 2003, 38-43.)NIST Spectranist ri  |
| 977 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 100801; Active phase: Polymethylsiloxane, (PMS-20000); Data type: Normal alkane RI; Authors: Cornwell, E.; Cordano, G., Nueva proposicion para predecir datos de retencion obtenidos mediante cromatografia de gases de hidrocarburos derivados de las naftas, Revista de la Sociedad Quimica de Mexico, 47(1), 2003, 38-43.)NIST Spectranist ri  |
| 981 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 160 C; CAS no: 100801; Active phase: OV-1; Data type: Normal alkane RI; Authors: Orav, A.; Kailas, T.; Muurisepp, M.; Kann, J., Composition of the oil from waste tires. 2. Fraction boiling at 160-180 0C, Proc. Estonian Acad. Sci. Chem., 48(3), 1999, 136-140.)NIST Spectranist ri  |
| 976 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 50 m; Column type: Capillary; Heat rate: 1 K/min; Start T: 30 C; End T: 100 C; Start time: 6 min; CAS no: 100801; Active phase: OV-101; Carrier gas: Helium; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Orav, A.; Kailas, T.; Muurisepp, M.; Kann, J., Composition of the oil from waste tires. 1. Fraction boiling at yp to 160 0C, Proc. Estonian Acad. Sci. Chem., 48(1), 1999, 30-39.)NIST Spectranist ri  |
| 991 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 280 C; End time: 30 min; CAS no: 100801; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Wang, S.-F.; Liu, B.-Z.; Sun, K.-J.; Su, Q.-D., Gas chromatographic-mass spectrometric determination of polycyclic aromatic hydrocarbons formed during the pyrolysis of phenylalanine, J. Chromatogr. A, 1025, 2004, 255-261.)NIST Spectranist ri  |
| 1348 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 100801; Active phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Cornwell, E.; Cordano, G., Nueva proposicion para predecir datos de retencion obtenidos mediante cromatografia de gases de hidrocarburos derivados de las naftas, Revista de la Sociedad Quimica de Mexico, 47(1), 2003, 38-43.)NIST Spectranist ri  |

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

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| --- | --- |
| Density:  | 0. 9±0. 1 g/cm 3  |
| Boiling Point:  | 170. 0±10. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 2. 0±0. 1 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 39. 0±0. 8 kJ/mol  |
| Flash Point:  | 51. 1±0. 0 °C  |
| Index of Refraction:  | 1. 551  |
| Molar Refractivity:  | 42. 0±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 1  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 3. 16  |
| ACD/LogD (pH 5. 5):  | 3. 46  |
| ACD/BCF (pH 5. 5):  | 251. 43  |
| ACD/KOC (pH 5. 5):  | 1818. 99  |
| ACD/LogD (pH 7. 4):  | 3. 46  |
| ACD/BCF (pH 7. 4):  | 251. 43  |
| ACD/KOC (pH 7. 4):  | 1818. 99  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 16. 7±0. 5 10 -24 cm 3  |
| Surface Tension:  | 30. 7±3. 0 dyne/cm  |
| Molar Volume:  | 131. 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) = 3. 44Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 168. 39 (Adapted Stein & Brown method)Melting Pt (deg C): -30. 07 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 08 (Mean VP of Antoine & Grain methods)MP (exp database): -86. 3 deg CBP (exp database): 164 deg CVP (exp database): 1. 70E+00 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 117. 1log Kow used: 3. 44 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 89 mg/L (25 deg C)Exper. Ref: YAWS, CL ET AL (1990)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 54. 156 mg/LWat Sol (Exper. database match) = 89. 00Exper. Ref: YAWS, CL ET AL (1990)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 3. 05E-003 atm-m3/moleGroup Method: 3. 01E-003 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 762E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 44 (KowWin est)Log Kaw used: -0. 904 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 344Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7460Biowin2 (Non-Linear Model) : 0. 8708Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8632 (weeks )Biowin4 (Primary Survey Model) : 3. 6087 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4535Biowin6 (MITI Non-Linear Model): 0. 4968Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 1380Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 0. 5907BioHC Half-Life (days) : 3. 8971Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 227 Pa (1. 7 mm Hg)Log Koa (Koawin est ): 4. 344Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 32E-008 Octanol/air (Koa) model: 5. 42E-009 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 4. 78E-007 Mackay model : 1. 06E-006 Octanol/air (Koa) model: 4. 34E-007 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 31. 2216 E-12 cm3/molecule-secHalf-Life = 0. 343 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 4. 111 HrsOzone Reaction: OVERALL Ozone Rate Constant = 2. 100000 E-17 cm3/molecule-secHalf-Life = 0. 546 Days (at 7E11 mol/cm3)Half-Life = 13. 097 HrsFraction sorbed to airborne particulates (phi): 7. 68E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 838. 6Log Koc: 2. 924 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 = 1. 951 (BCF = 89. 24)log Kow used: 3. 44 (estimated)Volatilization from Water: Henry LC: 0. 00301 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 321 hoursHalf-Life from Model Lake : 105. 6 hours (4. 398 days)Removal In Wastewater Treatment: Total removal: 58. 19 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 8. 66 percentTotal to Air: 49. 43 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 1. 31 5. 05 1000 Water 21 360 1000 Soil 76. 9 720 1000 Sediment 0. 824 3. 24e+003 0 Persistence Time: 305 hr

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