

# [Butyl isobutyrate c8h16o2 structure](https://assignbuster.com/butyl-isobutyrate-c8h16o2-structure/)

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* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 8 H 16 O 2  |
| Average mass  | 144. 211 Da  |
| Density  | 0. 9±0. 1 g/cm 3  |
| Boiling Point  | 156. 3±8. 0 °C at 760 mmHg  |
| Flash Point  | 46. 7±8. 3 °C  |
| Molar Refractivity  | 40. 8±0. 3 cm 3  |
| Polarizability  | 16. 2±0. 5 10 -24 cm 3  |
| Surface Tension  | 26. 3±3. 0 dyne/cm  |
| Molar Volume  | 164. 4±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| <25 °CFooDBFDB019968  |

## Experimental Boiling Point:

|  |
| --- |
| 155-156 °C (Literature)LabNetworkLN00196136  |
| 155 °CFooDBFDB019968  |

## Experimental Flash Point:

|  |
| --- |
| 43 °CLabNetworkLN00196136  |

## Experimental Refraction Index:

|  |
| --- |
| 20FooDBFDB019968  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 920 (estimated with error: 47)NIST Spectramainlib\_4078, replib\_285039, replib\_228837, replib\_249302  |
| 935 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 210 C; Start time: 4 min; CAS no: 97870; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Takeoka, G. R.; Flath, R. A.; Mon, T. R.; Teranishi, R.; Guentert, M., Volatile Constituents of Apricot (Prunus armeniaca), J. Agric. Food Chem., 38(2), 1990, 471-477.)NIST Spectranist ri  |
| 936 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 100 C; CAS no: 97870; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb W AW (60-80 mesh); Data type: Kovats RI; Authors: Chastrette, M.; Heintz, M.; Druilhe, A.; Lefort, D., Analyse chromatographique d’esters aliphatiques satures. Relations retention-structure et prevision de la retention, Bull. Soc. Chim. Fr., , 1974, 1852-1856., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 210 C; Start time: 4 min; CAS no: 97870; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Takeoka, G. R.; Flath, R. A.; Mon, T. R.; Teranishi, R.; Guentert, M., Volatile Constituents of Apricot (Prunus armeniaca), J. Agric. Food Chem., 38(2), 1990, 471-477.)NIST Spectranist ri  |
| 943 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 210 C; Start time: 4 min; CAS no: 97870; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Takeoka, G. R.; Flath, R. A.; Mon, T. R.; Teranishi, R.; Guentert, M., Volatile Constituents of Apricot (Prunus armeniaca), J. Agric. Food Chem., 38(2), 1990, 471-477.)NIST Spectranist ri  |
| 944 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 210 C; Start time: 4 min; CAS no: 97870; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Takeoka, G. R.; Flath, R. A.; Mon, T. R.; Teranishi, R.; Guentert, M., Volatile Constituents of Apricot (Prunus armeniaca), J. Agric. Food Chem., 38(2), 1990, 471-477.)NIST Spectranist ri  |
| 937 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 15 m; Column type: Capillary; Start T: 80 C; CAS no: 97870; Active phase: OV-101; Data type: Kovats RI; Authors: Komarek, K.; Hornova, L.; Horna, A.; Churacek, J., Glass capillary gas chromatography of homologous series of esters. IV. Separation of homologous series of certain halogenopropyl esters of aliphatic carboxylic acids on OV-101, J. Chromatogr., 281, 1983, 299-303.)NIST Spectranist ri  |
| 931 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 12 ft; Column type: Packed; Start T: 150 C; CAS no: 97870; Active phase: SE-30; Substrate: Celaton (62-72 mesh); Data type: Kovats RI; Authors: Ashes, J. R.; Haken, J. K., Gas chromatography of homologous esters. VI. Structure-retention increments of aliphatic esters, J. Chromatogr., 101, 1974, 103-123., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 12 ft; Column type: Packed; Start T: 150 C; CAS no: 97870; Active phase: SE-30; Substrate: Chromosorb W AW DMCS; Data type: Kovats RI; Authors: Haken, J. K.; Srisukh, D., Gas chromatography of homologous esters. XV. Molecular retention indices of aliphatic esters, J. Chromatogr., 219, 1981, 45-52., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; CAS no: 97870; Active phase: SE-30; Data type: Kovats RI; Authors: Chretien, J. R.; Dubois, J-E., Topological Analysis: A Technique for the Physico-Chemical Exploitation of Retention Data in Gas-Liquid Chromatography, J. Chromatogr., 158, 1978, 43-56.)NIST Spectranist ri  |
| 933 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 12 ft; Column type: Packed; Start T: 150 C; CAS no: 97870; Active phase: SE-30; Substrate: Celite 560; Data type: Kovats RI; Authors: Germaine, R. W.; Haken, J. K., Gas chromatography of homologous esters. Part 1. Simple aliphatic esters, J. Chromatogr., 43, 1969, 33-42., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Packed; Start T: 150 C; CAS no: 97870; Active phase: OV-1; Data type: Kovats RI; Authors: Ashes, J. R.; Haken, J. K., Gas chromatography of homologous esters. Part V. Retention of aliphatic esters on non-polar, donar and acceptor stationary phases, J. Chromatogr., 60, 1971, 33-44.)NIST Spectranist ri  |
| 952 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 100 C; CAS no: 97870; Active phase: SE-30; Substrate: Chromosorb W; Data type: Kovats RI; Authors: Zarazir, D.; Chovin, P.; Guiochon, G., Identification of hydroxylic compounds and their derivatives by gas chromatography, Chromatographia, 3, 1970, 180-195.)NIST Spectranist ri  |
| 894 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 25 m; Column type: Packed; Start T: 130 C; CAS no: 97870; Active phase: Apiezon L; Substrate: Celite; Data type: Kovats RI; Authors: Wehrli, A.; Kovats, E., Gas-chromatographische Charakterisierung ogranischer Verbindungen. Teil 3: Berechnung der Retentionsindices aliphatischer, alicyclischer und aromatischer Verbindungen, Helv. Chim. Acta, 7, 1959, 2709-2736., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 130 C; CAS no: 97870; Active phase: Apiezon L; 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  |
| 895 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 120 C; CAS no: 97870; 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  |
| 908 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 160 C; CAS no: 97870; 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  |
| 891 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 70 C; CAS no: 97870; Active phase: Squalane; Substrate: Chromosorb G; Data type: Kovats RI; Authors: Mira, J. M.; Sanchez, L. G., Polarity of the Gas Chromatographic Stationary Phases and Retention Indices of Aliphatic Esters, Ketones and Alcohols, Anal. Chim. Acta., 50, 1970, 315-321.)NIST Spectranist ri  |
| 898 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 25 m; Column type: Packed; Start T: 190 C; CAS no: 97870; Active phase: Apiezon L; Substrate: Celite; Data type: Kovats RI; Authors: Wehrli, A.; Kovats, E., Gas-chromatographische Charakterisierung ogranischer Verbindungen. Teil 3: Berechnung der Retentionsindices aliphatischer, alicyclischer und aromatischer Verbindungen, Helv. Chim. Acta, 7, 1959, 2709-2736.)NIST Spectranist ri  |
| 1149 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 60 C; End T: 200 C; Start time: 10 min; CAS no: 97870; Active phase: DB-Wax; Carrier gas: N2; Data type: Kovats RI; Authors: Umano, K.; Shoji, A.; Hagi, Y.; Shibamoto, T., Volatile constituents of peel of quince fruit, Cydonia oblonga Miller, J. Agric. Food Chem., 34(4), 1986, 593-596.)NIST Spectranist ri  |
| 1145 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 100 C; CAS no: 97870; Active phase: Carbowax 20M; Substrate: Chromosorb WAW (60-80 mesh); Data type: Kovats RI; Authors: Chastrette, M.; Heintz, M.; Druilhe, A.; Lefort, D., Analyse chromatographique d’esters aliphatiques satures. Relations retention-structure et prevision de la retention, Bull. Soc. Chim. Fr., , 1974, 1852-1856.)NIST Spectranist ri  |
| 1197 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 2 m; Column type: Packed; Start T: 100 C; CAS no: 97870; Active phase: Carbowax 20M; Substrate: Chromosorb W; Data type: Kovats RI; Authors: Zarazir, D.; Chovin, P.; Guiochon, G., Identification of hydroxylic compounds and their derivatives by gas chromatography, Chromatographia, 3, 1970, 180-195.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

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| --- |
| 934 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 30 C; End T: 210 C; CAS no: 97870; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Kumazawa, K.; Itobe, T.; Nishimura, O.; Hamaguchi, T., A new approach to estimate the in-mouth release characteristics of odorants in chewing gum, Food Science and Technology Research, 14(3), 2008, 269-276.)NIST Spectranist ri  |
| 931 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 97870; Active phase: SE-30; Data type: Normal alkane RI; Authors: Liu, F.; Liang, Y.; Cao, C.; Zhou, N., QSPR study of GC retention indices for saturated esters on seven stationary phases based on novel topological indices, Talanta, 72, 2007, 1307-1315.)NIST Spectranist ri  |
| 939 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 28 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 80 C; End T: 200 C; CAS no: 97870; Active phase: OV-101; Data type: Normal alkane RI; Authors: Anker, L. S.; Jurs, P. C.; Edwards, P. A., Quantitative structure-retention relationship studies of odor-active aliphatic compounds with oxygen-containing functional groups, Anal. Chem., 62, 1990, 2676-2684., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 97870; 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  |
| 945 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; Heat rate: 2 K/min; Start T: 70 C; End T: 170 C; CAS no: 97870; Active phase: SE-30; Carrier gas: Helium; Data type: Normal alkane RI; Authors: Alves, S.; Jennings, W. G., Volatile composition of certain Amazonian fruits, Food Chem., 4(2), 1979, 149-159.)NIST Spectranist ri  |
| 944 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Packed; Start T: 70 C; CAS no: 97870; Active phase: SE-30; Data type: Normal alkane RI; Authors: Yabumoto, K.; Jennings, W. G.; Yamaguchi, M., Gas chromatographic retention as identification criteria, Anal. Biochem., 78, 1977, 244-251.)NIST Spectranist ri  |
| 911 (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: 50 C; End T: 230 C; End time: 10 min; Start time: 4 min; CAS no: 97870; Active phase: HP-5 MS; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Forero, M. D.; Quijano, C. E.; Pino, J. A., Volatile compounds of Chile pepper (Capsicum annuum L. var. glabriusculum) at two ripening stages, Flavour Fragr. J., 24, 2008, 25-30.)NIST Spectranist ri  |
| 1129 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 20 mm; Column length: 50 m; Column type: Capillary; Description: 70 0C (1 min) ^ 3 0C/min -> 142 0C ^ 5 0C/min -> 225 0C (10 min); CAS no: 97870; Active phase: FFAP; Carrier gas: Helium; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Ortiz, A.; Echeverra, G.; Graell, J.; Lara, I., Calcium dips enhance volatile emission of cold-stored “ Fuji Kiki-8” apples, J. Agric. Food Chem., 57(11), 2009, 4931-4938.)NIST Spectranist ri  |
| 1149 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 30 C; End T: 210 C; CAS no: 97870; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Kumazawa, K.; Itobe, T.; Nishimura, O.; Hamaguchi, T., A new approach to estimate the in-mouth release characteristics of odorants in chewing gum, Food Science and Technology Research, 14(3), 2008, 269-276.)NIST Spectranist ri  |
| 1139 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 2 mm; Column length: 80 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 70 C; End T: 170 C; CAS no: 97870; Active phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Anker, L. S.; Jurs, P. C.; Edwards, P. A., Quantitative structure-retention relationship studies of odor-active aliphatic compounds with oxygen-containing functional groups, Anal. Chem., 62, 1990, 2676-2684., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 97870; 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  |
| 1159 (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: 60 C; End T: 220 C; End time: 10 min; Start time: 10 min; CAS no: 97870; Active phase: Innowax; Carrier gas: He; Data type: Normal alkane RI; Authors: Suleimenov, E. M.; Atazharova, G. A.; Demirchi, B.; Baser, K. H. C.; Adekenov, S. M., Essential oil composition of Artemisia Lercheana and A. Sieversiana of Kazakhstan flora, in Recent problems of development of new medicines of natural origin, Proceedings of symposium, St. Petersburg – Pushkin, 2003, 382-385.)NIST Spectranist ri  |
| 1147 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Packed; Start T: 100 C; CAS no: 97870; Active phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Yabumoto, K.; Jennings, W. G.; Yamaguchi, M., Gas chromatographic retention as identification criteria, Anal. Biochem., 78, 1977, 244-251.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 952 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Description: -20C (5min) => 10C/min => 100C => 4C/min => 200C => 10C/min => 280C; CAS no: 97870; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Eri, S.; Khoo, B. K.; Lech, J.; Hartman, T. G., Direct thermal desorption-gas chromatography and gas chromatography-mass spectrometry profiling of hop (Humulus lupulus L.) essential oils in support of varietal characterization, J. Agric. Food Chem., 48, 2000, 1140-1149.)NIST Spectranist ri  |
| 954 (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: 20 K/min; Start T: 50 C; End T: 220 C; End time: 2 min; Start time: 2 min; CAS no: 97870; Active phase: SPB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Balbontin, C.; Gaete-Eastman, C.; Vergara, M.; Herrera, R.; Moya-Leon, M. A., Treatment with 1-MCP and the role of ethylene in aroma development of mountain papaya fruit, Postharvest Biol. Technol., 43, 2007, 67-77.)NIST Spectranist ri  |
| 955 (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: 60 C; End T: 250 C; End time: 20 min; Start time: 2 min; CAS no: 97870; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Pino, J. A.; Mesa, J.; Munoz, Y.; Marti, M. P.; Marbot, R., Volatile components from mango (Mangifera indica L.) cultivars, J. Agric. Food Chem., 53, 2005, 2213-2223.)NIST Spectranist ri  |
| 1154 (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: 97870; 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  |

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

|  |  |
| --- | --- |
| Density:  | 0. 9±0. 1 g/cm 3  |
| Boiling Point:  | 156. 3±8. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 2. 9±0. 3 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 39. 3±3. 0 kJ/mol  |
| Flash Point:  | 46. 7±8. 3 °C  |
| Index of Refraction:  | 1. 411  |
| Molar Refractivity:  | 40. 8±0. 3 cm 3  |
| #H bond acceptors:  | 2  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 5  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 2. 65  |
| ACD/LogD (pH 5. 5):  | 2. 42  |
| ACD/BCF (pH 5. 5):  | 40. 51  |
| ACD/KOC (pH 5. 5):  | 492. 37  |
| ACD/LogD (pH 7. 4):  | 2. 42  |
| ACD/BCF (pH 7. 4):  | 40. 51  |
| ACD/KOC (pH 7. 4):  | 492. 37  |
| Polar Surface Area:  | 26 Å 2  |
| Polarizability:  | 16. 2±0. 5 10 -24 cm 3  |
| Surface Tension:  | 26. 3±3. 0 dyne/cm  |
| Molar Volume:  | 164. 4±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. 76Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 157. 09 (Adapted Stein & Brown method)Melting Pt (deg C): -43. 92 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 3. 18 (Mean VP of Antoine & Grain methods)MP (exp database): 8 at 25 deg C : 3. 709E-002 L/mol-secKb Half-Life at pH 8: 216. 263 days Kb Half-Life at pH 7: 5. 921 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 1. 421 (BCF = 26. 39)log Kow used: 2. 76 (estimated)Volatilization from Water: Henry LC: 0. 000974 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 947 hoursHalf-Life from Model Lake : 121. 9 hours (5. 081 days)Removal In Wastewater Treatment: Total removal: 31. 55 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 3. 28 percentTotal to Air: 28. 18 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 9. 92 46. 7 1000 Water 25 208 1000 Soil 64. 9 416 1000 Sediment 0. 216 1. 87e+003 0 Persistence Time: 216 hr

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