

# [1-chloro-4-methoxybutane c5h11clo structure](https://assignbuster.com/1-chloro-4-methoxybutane-c5h11clo-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 5 H 11 ClO  |
| Average mass  | 122. 593 Da  |
| Density  | 1. 0±0. 1 g/cm 3  |
| Boiling Point  | 138. 3±23. 0 °C at 760 mmHg  |
| Flash Point  | 47. 8±17. 9 °C  |
| Molar Refractivity  | 31. 8±0. 3 cm 3  |
| Polarizability  | 12. 6±0. 5 10 -24 cm 3  |
| Surface Tension  | 25. 4±3. 0 dyne/cm  |
| Molar Volume  | 128. 8±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 819 (estimated with error: 89)NIST Spectramainlib\_153869, replib\_46403  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 840. 3 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; CAS no: 17913187; Active phase: Squalane; Data type: Normal alkane RI; Authors: Keiko, V. V.; Prokop’ev, B. V.; Kuz’menko, L. P.; Kalinina, N. A.; Modonov, V. B., The use of an additive scheme of calculation of the indices of retention in gas-liquid chromatography communication. 3. Some regularities in the manifestation of the inductive effect, Izv. Akad. Nauk Kaz. SSR Ser. Khim., 12, 1972, 2629-2633, In original 2697-2702.)NIST Spectranist ri  |
| 847. 3 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; CAS no: 17913187; Active phase: Apiezon L; Data type: Normal alkane RI; Authors: Keiko, V. V.; Prokop’ev, B. V.; Kuz’menko, L. P.; Kalinina, N. A.; Modonov, V. B., The use of an additive scheme of calculation of the indices of retention in gas-liquid chromatography communication. 3. Some regularities in the manifestation of the inductive effect, Izv. Akad. Nauk Kaz. SSR Ser. Khim., 12, 1972, 2629-2633, In original 2697-2702.)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:  | 138. 3±23. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 8. 4±0. 2 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 36. 0±3. 0 kJ/mol  |
| Flash Point:  | 47. 8±17. 9 °C  |
| Index of Refraction:  | 1. 408  |
| Molar Refractivity:  | 31. 8±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 4  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 1. 33  |
| ACD/LogD (pH 5. 5):  | 1. 58  |
| ACD/BCF (pH 5. 5):  | 9. 35  |
| ACD/KOC (pH 5. 5):  | 172. 36  |
| ACD/LogD (pH 7. 4):  | 1. 58  |
| ACD/BCF (pH 7. 4):  | 9. 35  |
| ACD/KOC (pH 7. 4):  | 172. 36  |
| Polar Surface Area:  | 9 Å 2  |
| Polarizability:  | 12. 6±0. 5 10 -24 cm 3  |
| Surface Tension:  | 25. 4±3. 0 dyne/cm  |
| Molar Volume:  | 128. 8±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) = 1. 79Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 136. 33 (Adapted Stein & Brown method)Melting Pt (deg C): -54. 48 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 7. 52 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 2882log Kow used: 1. 79 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 7173. 7 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 11E-004 atm-m3/moleGroup Method: 2. 87E-005 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 209E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 79 (KowWin est)Log Kaw used: -1. 537 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 3. 327Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2304Biowin2 (Non-Linear Model) : 0. 0177Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7464 (weeks-months)Biowin4 (Primary Survey Model) : 3. 5605 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5481Biowin6 (MITI Non-Linear Model): 0. 4944Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 5886Ready 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): 924 Pa (6. 93 mm Hg)Log Koa (Koawin est ): 3. 327Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 25E-009 Octanol/air (Koa) model: 5. 21E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 17E-007 Mackay model : 2. 6E-007 Octanol/air (Koa) model: 4. 17E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 12. 7084 E-12 cm3/molecule-secHalf-Life = 0. 842 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 10. 100 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 1. 89E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 14. 95Log Koc: 1. 175 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. 682 (BCF = 4. 804)log Kow used: 1. 79 (estimated)Volatilization from Water: Henry LC: 2. 87E-005 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 23. 72 hoursHalf-Life from Model Lake : 351. 6 hours (14. 65 days)Removal In Wastewater Treatment: Total removal: 3. 61 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 97 percentTotal to Air: 1. 55 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 1. 65 20. 2 1000 Water 35. 1 900 1000 Soil 63. 2 1. 8e+003 1000 Sediment 0. 109 8. 1e+003 0 Persistence Time: 627 hr

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