1-chloro-4-methoxybutane c5h11clo structure

Contents

Molecular Formula	$C_5H_{11}ClO$
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	128. 8±3. 0

Volume cm ^{3}

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

- **Retention Index (Kovats):**

  819

  (estimated

  with error:

  89)NIST

  Spectramainl

  ib_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

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scheme of

calculation of

the indices of

retention in

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(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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