2,3,4,5,6,7-hexahydro-1h-indene c9h14 structure

ASSIGN BUSTER

Contents

Molecular Formula	C_9H_{14}
Average mass	122. 207 Da
Density	0. 9±0. 1 g/cm ^{3}
Boiling Point	175. 8±0. 0 °C at 760 mmHg
Flash Point	43. 0±13. 0 °C
Molar Refractivity	39. 1±0. 4 cm ^{3}
Polarizability	15. 5±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	30. 3±5. 0 dyne/cm
Molar Volume	132. 8±5. 0 cm ^{3}

- **Retention Index (Kovats):**

  1020 (estimated with error: 39)NIST Spectramainlib_197586

- **Retention Index (Linear):**

  1001 (Program type: Ramp; Column cl... (show more)ass: Standard non-p Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capill rate: 1 K/min; Start T: 30 C; End T: 220 C; CAS no: 695909; Active phase: DH; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Auth White, C. M.; Hackett, J.; Anderson, R. R.; Kail, S.; Spock, P. S., Linear temperature programmed retention indices of gasoline range hydrocarbo chlorinated hydrocarbons on cross-linked polydimethylsiloxane, J. Hi. Res Chromatogr., 15, 1992, 105-120.)NIST Spectranist ri

1008. 6 (Program type: Ramp; Column cl... (show more)ass: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 2 K/min; Start T: 40 C; End T: 310 C; CAS no: 695909; Active p DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; A Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c. c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10), 1436-1451., Program type: Ramp; Column cl... (show more)ass: Semi-sta non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty Capillary; Heat rate: 2 K/min; Start T: 40 C; End T: 310 C; CAS no: 69590 phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Line Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed retention indices for GC and GC-MS of hydroc fuels and simulated distillation GC of heavy oils, in Analytical advances fo hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publish New York, 2003, 147-193.)NIST Spectranist ri

1009. 9 (Program type: Ramp; Column cl... (show more)ass: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 4 K/min; Start T: 40 C; End T: 310 C; Start time: 5 min; CAS no 695909; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; type: Linear RI; Authors: Lai, W.-C.; Song, C., Temperature-programmed indices for g. c. and g. c.-m. s. analysis of coal- and petroleum-derived liq fuels, Fuel, 74(10), 1995, 1436-1451., Program type: Ramp; Column cl... more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Colum 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 31 Start time: 5 min; CAS no: 695909; Active phase: DB-5; Carrier gas: He; P

thickness: 0. 25 um; Data type: Linear RI; Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed re indices for GC and GC-MS of hydrocarbon fuels and simulated distillation heavy oils, in Analytical advances for hydrocarbon research, Hsu, C. S., e Kluwer Academic/Plenum Publishers, New York, 2003, 147-193.)NIST Spe ri

1011. 4 (Program type: Ramp; Column cl... (show more)ass: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 4 K/min; Start T: 40 C; End T: 310 C; CAS no: 695909; Active p DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; A Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c. c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10), 1436-1451., Program type: Ramp; Column cl... (show more)ass: Semi-sta non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 310 C; CAS no: 695909 phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Line Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed retention indices for GC and GC-MS of hydroc fuels and simulated distillation GC of heavy oils, in Analytical advances fo hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publish New York, 2003, 147-193.)NIST Spectranist ri

1014. 8 (Program type: Ramp; Column cl... (show more)ass: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 6 K/min; Start T: 40 C; End T: 310 C; CAS no: 695909; Active p

DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; A

Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c.

c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10),

1436-1451., Program type: Ramp; Column cl... (show more)ass: Semi-sta

non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty

Capillary; Heat rate: 6 K/min; Start T: 40 C; End T: 310 C; CAS no: 69590

phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Line

Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7.

Temperature-programmed retention indices for GC and GC-MS of hydroc

fuels and simulated distillation GC of heavy oils, in Analytical advances fo

hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publish

New York, 2003, 147-193.)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:	175. 8±0. 0 °C at 760 mmHg
Vapour Pressure:	1. 5±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	39. 5±0. 8 kJ/mol
Flash Point:	43. 0±13. 0 °C
Index of Refraction:	1. 500
Molar Refractivity:	39. 1±0. 4 cm ^{3}

#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	3. 95
ACD/LogD (pH 5. 5):	3. 59
ACD/BCF (pH 5. 5):	313. 88
ACD/KOC (pH 5. 5):	2131. 99
ACD/LogD (pH 7. 4):	3. 59
ACD/BCF (pH 7. 4):	313. 88
ACD/KOC (pH 7. 4):	2131. 99
Polar Surface Area:	0 Å ^{2}
Polarizability:	15. 5±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	30. 3±5. 0 dyne/cm
Molar Volume:	132. 8±5. 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. 86Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 167. 90 (Adapted Stein & Brown method)Melting Pt (deg C): -19. 00 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 3 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 14. 46log Kow used: 3. 86 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 10. 312 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : IncompleteGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 558E-002 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Can Not Estimate (can not calculate HenryLC)Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6894Biowin2 (Non-Linear Model) : 0. 7813Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9291 (weeks)Biowin4 (Primary Survey Model) : 3. 6714 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4866Biowin6 (MITI Non-Linear Model): 0. 6577Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 0040Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 1. 6928BioHC Half-Life (days) : 49. 2984Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 280 Pa (2. 1 mm Hg)Log Koa (): not availableKp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 07E-008 Octanol/air (Koa) model: not availableFraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 87E-007 Mackay model : 8. 57E-007 Octanol/air (Koa) model: not availableAtmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 8. 3652 E-12 cm3/molecule-secHalf-Life = 1. 279 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 15. 343 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 6. 22E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 996. 2Log Koc: 2. 998 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 = 2. 272 (BCF = 187. 1)log Kow used: 3. 86 (estimated)Volatilization from Water: Henry LC: 0. 0256 atm-m3/mole (calculated from VP/WS)Half-Life from Model River: 1. 153 hoursHalf-Life from Model Lake : 105. 3 hours (4. 387 days)Removal In Wastewater Treatment: Total removal: 91. 90 percentTotal biodegradation: 0. 08 percentTotal sludge adsorption: 14. 61 percentTotal to Air: 77. 22 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 9. 29 30. 7 1000 Water 27. 2 360 1000 Soil 60. 9 720 1000 Sediment 2. 57 3. 24e+003 0 Persistence Time: 227 hr

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