3-ethyl-2,5-dimethylhexane c10h22 structure

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Contents

Molecular Formula	$C_{10}H_{22}$
Average mass	142. 282 Da
Density	0. 7±0. 1 g/cm ^{3}
Boiling Point	153. 5±7. 0 °C at 760 mmHg
Flash Point	39. 5±11. 7 °C
Molar Refractivity	48. 3±0. 3 cm ^{3}
Polarizability	19. 1±0. 5 10^{-24} cm ^{3}
Surface Tension	22. 1±3. 0 dyne/cm
Molar	194. 7±3. 0

Volume cm ^{3}

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

Retention Index (Kovats):

823 (estimated with error: 39)NIST Spectramainlib_ 154912

891 (Program type: Isothermal; Col... (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 300 ft; Column type:

Capillary; Start T: 60 C; CAS no: 52897048; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Matukuma, A., Retention indices of alkanes through C10 and alkenes through C8 and relation between boiling points and retention data, Gas Chromatogr., Int. Symp. Anal. Instrum. Div Instrum Soc. Amer., 7, 1969, 55-75., Program

type:
Isothermal;
Col… (show
more)umn
class: Semi-
standard non-
polar; Column
type: Capillary;
Start T: 100 C;
CAS no:
52897048;
Active phase:
Squalane; Data
type: Kovats RI;
Authors:
Heinzen, V. E.
F.; Soares, M.
F.; Yunes, R. A.,
Semi-empirical
topological
method for the
prediction of
the
chromatographi
c retention of
cis- and trans-

alkene isomers and alkanes, J. Chromatogr. A, 849, 1999, 495-506.)NIST Spectranist ri

891. 4 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 60 C; CAS no: 52897048; Active phase: Squalane; Data type: Kovats RI; Authors: Chretien, J. R.; Dubois, J.-E., New

Perspectives in the Prediction of Kovats Indices, J. Chromatogr., 126, 1976, 171-189.)NIST Spectranist ri

- **Retention Index (Normal Alkane):**

  891 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 52897048; Active phase: OV-101; Data type: Normal alkane RI; Authors: Du, Y.; Liang, Y., Data

mining for seeking accurate quantitative relationship between molecular structure and GC retention indices of alkanes by projection pursuit, Comput. Biol. Chem., 27, 2003, 339-353., Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 52897048; Active phase:

Polydimethyl
siloxane; Data
type: Normal
alkane RI;
Authors: Junkes,
B. S.; Castanho,
R. D. M.;
Amboni, C.;
Yunes, R. A.;
Heinzen, V. E.
F.,
Semiempirical
Topological
Index: A Novel
Molecular
Descriptor for
Quantitative
Structure-
Retention
Relationship
Studies,
Internet
Electronic
Journal of
Molecular
Design, 2(1),

2003, 33-

49.)NIST

Spectranist ri

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

Density:	0. 7±0. 1 g/cm ^{3}
Boiling Point:	153. 5±7. 0 °C at 760 mmHg
Vapour Pressure:	4. 3±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	37. 4±0. 8 kJ/mol
Flash Point:	39. 5±11. 7 °C
Index of Refraction:	1. 410
Molar Refractivity:	48. 3±0. 3 cm ^{3}
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	4
#Rule of 5 Violations:	1
ACD/LogP:	5. 52

ACD/LogD (pH 5. 5):	4. 75
ACD/BCF (pH 5. 5):	2415. 10
ACD/KOC (pH 5. 5):	9185. 46
ACD/LogD (pH 7. 4):	4. 75
ACD/BCF (pH 7. 4):	2415. 10
ACD/KOC (pH 7. 4):	9185. 46
Polar Surface Area:	0 Å ^{2}
Polarizability:	19. 1±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	22. 1±3. 0 dyne/cm
Molar Volume:	194. 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) = 5. 03Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 124. 32 (Adapted Stein & Brown method)Melting Pt (deg C): -78. 39 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 4. 28 (Mean VP of Antoine & Grain methods)BP (exp database): 154. 1 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1. 2log Kow used: 5. 03 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 43165 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 30E+000 atm-m3/moleGroup Method: 1. 17E+001 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 6. 678E-001 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 03 (KowWin est)Log Kaw used: 2. 336 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 694Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6798Biowin2 (Non-Linear Model) : 0. 7287Expert Survey

Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8847 (weeks)Biowin4 (Primary Survey Model) : 3. 6425 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2377Biowin6 (MITI Non-Linear Model): 0. 2839Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 0073Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 1. 0111BioHC Half-Life (days) : 10. 2591Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 523 Pa (3. 92 mm Hg)Log Koa (Koawin est): 2. 694Kp (particle/gas partition coef. (m3/ug)): Mackay model : 5. 74E-009 Octanol/air (Koa) model: 1. 21E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 07E-007 Mackay model : 4. 59E-007 Octanol/air (Koa) model: 9. 71E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 11. 7808 E-12 cm3/molecule-secHalf-Life = 0. 908 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 10. 895 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 3. 33E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1137Log Koc: 3. 056 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 = 3. 175 (BCF = 1495)log Kow used: 5. 03 (estimated)Volatilization from Water: Henry LC: 5. 3 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 217 hoursHalf-Life from Model Lake : 113. 3 hours (4. 721 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 99. 97 percentTotal biodegradation: 0. 15 percentTotal sludge adsorption: 48. 55 percentTotal to Air: 51. 27 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 11. 2 21. 8 1000 Water 35. 7 360 1000 Soil 9. 59 720 1000 Sediment 43. 5 3. 24e+003 0 Persistence Time: 169 hr

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