2,2,4,5-tetramethylhexane c10h22 structure

Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_{10}H_{22}$
Average mass	142. 282 Da
Density	0. 7±0. 1 g/cm ^{3}
Boiling Point	147. 7±7. 0 °C at 760 mmHg
Flash Point	36. 4±11. 7 °C
Molar Refractivity	48. 3±0. 3 cm ^{3}
Polarizability	19. 1±0. 5 10^{-24} cm ^{3}
Surface Tension	21. 8±3. 0 dyne/cm
Molar	194. 4±3. 0

Volume cm ^{3}

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

Retention Index (Kovats):

872 (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: 16747425; 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: 16747425; 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 chromatographic retention of cis- and trans-alkene isomers and alkanes, J. Chromatogr. A, 849, 1999, 495-506.)NIST

Spectranist ri

870 (Program type: Isothermal; Col... (show more)umn class: Semi-standard non-polar; Column type: Capillary; CAS no: 16747425; Active phase: Squalane; Data type: Kovats RI; Authors: Korol, A. N.; Lysyuk, L. S., A New Thermodynamic Method for Calculating the Retention Indices of Isoalkanes on Squalane,

Theor. Exp.

Chem. (Engl.

Transl.), 16(6),

1980, 577-584,

In original 792-

800.)NIST

Spectranist ri

872. 1

(Program type:

Isothermal;

Col... (show

more)umn

class: Semi-

standard non-

polar; Column

type: Capillary;

Start T: 60 C;

CAS no:

16747425;

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):**

  872 (Program

  type: Ramp;

  Column cl...

  (show

  more)ass:

  Standard non-

  polar; Column

  type: Capillary;

  CAS no:

  16747425;

  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: 16747425;

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:	147. 7±7. 0 °C at 760 mmHg
Vapour Pressure:	5. 5±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	36. 9±0. 8 kJ/mol
Flash Point:	36. 4±11. 7 °C
Index of Refraction:	1. 411
Molar Refractivity:	48. 3±0. 3 cm ^{3}
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	1

ACD/LogP:	5. 34
ACD/LogD (pH 5. 5):	4. 51
ACD/BCF (pH 5. 5):	1579. 91
ACD/KOC (pH 5. 5):	6779. 20
ACD/LogD (pH 7. 4):	4. 51
ACD/BCF (pH 7. 4):	1579. 91
ACD/KOC (pH 7. 4):	6779. 20
Polar Surface Area:	0 $Å^2$
Polarizability:	19. 1±0. 5 10^{-24} cm^3
Surface Tension:	21. 8±3. 0 dyne/cm
Molar Volume:	194. 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) = 4. 99Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 115. 09 (Adapted Stein & Brown method)Melting Pt (deg C): -72. 37 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 5. 63 (Mean VP of Antoine & Grain methods)BP (exp database): 147. 9 deg CVP (exp database): 6. 02E+00 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1. 292log Kow used: 4. 99 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 63395 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]: 8. 158E-001 atm-m3/moleLog Octanol-Air

Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 99 (KowWin est)Log Kaw used: 2. 336 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 654Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 4959Biowin2 (Non-Linear Model) : 0. 3241Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 6726 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4890 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3070Biowin6 (MITI Non-Linear Model): 0. 3023Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 2813Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 1. 2314BioHC Half-Life (days) : 17. 0357Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 803 Pa (6. 02 mm Hg)Log Koa (Koawin est): 2. 654Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 74E-009 Octanol/air (Koa) model: 1. 11E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 35E-007 Mackay model : 2. 99E-007 Octanol/air (Koa) model: 8. 85E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 7. 7380 E-12 cm3/molecule-secHalf-Life = 1. 382 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 16. 587 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 17E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 840. 2Log Koc: 2. 924 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. 146 (BCF = 1398)log Kow used: 4. 99 (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. 14 percentTotal sludge adsorption: 47. 67 percentTotal to Air: 52. 15 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 9. 37 33. 2 1000 Water 26. 4 900 1000 Soil 5. 25 1. 8e+003 1000 Sediment 59 8. 1e+003 0 Persistence Time: 290 hr

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