

2,2,7,7-
tetramethyloctane
c12h26 structure



**ASSIGN
BUSTER**

Contents

- Retention Index (Linear):

Molecular Formula	C ₁₂ H ₂₆
Average mass	170.335 Da
Density	0.8±0.1 g/cm ³
Boiling Point	184.7±7.0 °C at 760 mmHg
Flash Point	62.3±11.7 °C
Molar Refractivity	57.6±0.3 cm ³
Polarizability	22.8±0.5 10 ⁻²⁴ cm ³
Surface Tension	23.6±3.0 dyne/cm
Molar Volume	226.7±3.0 cm ³

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

- **Retention Index (Kovats):**

1045 (estimated with error: 39)NIST

Spectramainlib_113585

- **Retention Index (Linear):**

1038. 54 (Program type: Ramp; Column cl... (show more)ass: Standard n
polar; Column diameter: 0. 22 mm; Column length: 50 m; Column type: C
Heat rate: 1 K/min; Start T: -30 C; End T: 240 C; CAS no: 1071314; Active
Ultra-1; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Linear RI;
Haynes, P. C., Jr.; Pitzer, E. W., Disengaging solutes in shale- and petrole
derived jet fuels by altering GC programmed temperature rates, J. Hi. Re
Chromatogr. & Chromatogr. Comm., 8, 1985, 230-242.)NIST Spectranist

1039. 44 (Program type: Ramp; Column cl... (show more)ass: Standard n
polar; Column diameter: 0. 22 mm; Column length: 50 m; Column type: C
Heat rate: 2 K/min; Start T: -30 C; End T: 240 C; CAS no: 1071314; Active
Ultra-1; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Linear RI;
Haynes, P. C., Jr.; Pitzer, E. W., Disengaging solutes in shale- and petrole
derived jet fuels by altering GC programmed temperature rates, J. Hi. Re
Chromatogr. & Chromatogr. Comm., 8, 1985, 230-242.)NIST Spectranist

1039. 5 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0. 22 mm; Column length: 50 m; Column type: Capillary; Heat rate: 3 K/min; Start T: -30 C; End T: 240 C; CAS no: 1071314; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Linear RI; Authors: Haynes, P. C., Jr.; Pitzer, E. W., Disengaging solutes in shale- and petroleum-derived jet fuels by altering GC programmed temperature rates, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 8, 1985, 230-242.)NIST Spectranist

1013 (Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 20 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 60 C; End T: 240 C; End time: 15 min; Start time: 5 min; CAS no: 1071314; Active phase: HP-5MS; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Kallio, M.; Jussila, M.; Rissanen, T.; Anttila, P.; Hakola, K.; Reissell, A.; Vreuls, R.; Adahchour, M.; Hyotylainen, T., Comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry for the identification of organic compounds in atmospheric aerosols from coniferous forest, J. Chromatogr. A, 1125, 2006, 234-243.)NIST Spectranist ri

1035. 93 (Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0. 22 mm; Column length: 50 m; Column type: Capillary; Heat rate: 1 K/min; Start T: -30 C; End T: 240 C; CAS no: 1071314; Active phase: Ultra-2; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Linear RI; Authors: Haynes, P. C., Jr.; Pitzer, E. W., Disengaging solutes in shale- and petroleum-derived jet fuels by altering GC programmed temperature rates, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 8, 1985, 230-242.)NIST Spectranist

1036. 7 (Program type: Ramp; Column cl... (show more)ass: Semi-standard

polar; Column diameter: 0.22 mm; Column length: 50 m; Column type: C
Heat rate: 2 K/min; Start T: -30 C; End T: 240 C; CAS no: 1071314; Active
Ultra-2; Carrier gas: He; Phase thickness: 0.33 µm; Data type: Linear RI;
Haynes, P. C., Jr.; Pitzer, E. W., Disengaging solutes in shale- and petroleum
derived jet fuels by altering GC programmed temperature rates, J. Hi. Re
Chromatogr. & Chromatogr. Comm., 8, 1985, 230-242.)NIST Spectranist

1036.75 (Program type: Ramp; Column cl... (show more)ass: Semi-stand
polar; Column diameter: 0.22 mm; Column length: 50 m; Column type: C
Heat rate: 3 K/min; Start T: -30 C; End T: 240 C; CAS no: 1071314; Active
Ultra-2; Carrier gas: He; Phase thickness: 0.33 µm; Data type: Linear RI;
Haynes, P. C., Jr.; Pitzer, E. W., Disengaging solutes in shale- and petroleum
derived jet fuels by altering GC programmed temperature rates, J. Hi. Re
Chromatogr. & Chromatogr. Comm., 8, 1985, 230-242.)NIST Spectranist

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

Density:	0.8 ± 0.1 g/cm ³
Boiling Point:	184.7 ± 7.0 °C at 760 mmHg
Vapour Pressure:	1.0 ± 0.2 mmHg at 25°C
Enthalpy of Vaporization:	40.4 ± 0.8 kJ/mol
Flash Point:	62.3 ± 11.7 °C
Index of Refraction:	1.422

Molar Refractivity:	57.6 ± 0.3 cm ³
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	5
#Rule of 5 Violations:	1
ACD/LogP:	6.40
ACD/LogD (pH 5.5):	5.94
ACD/BCF (pH 5.5):	19129.98
ACD/KOC (pH 5.5):	40405.24
ACD/LogD (pH 7.4):	5.94
ACD/BCF (pH 7.4):	19129.98
ACD/KOC (pH 7.4):	40405.24
Polar Surface Area:	0 Å ²
Polarizability:	22.8 ± 0.5 10 ⁻²⁴ cm ³
Surface Tension:	23.6 ± 3.0 dyne/cm

Molar Volume: 226. 7±3. 0 cm³

Predicted data is generated using the US Environmental Protection Agency's
EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 6. 01Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 164. 64 (Adapted Stein & Brown method)Melting Pt (deg C): -30. 43 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 67 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 1305log Kow used: 6. 01 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 056084 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenry's Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 9. 35E+000 atm-m³/moleGroup Method: 1. 94E+001 atm-m³/moleHenry's LC [VP/WSol estimate using EPI values]: 4. 586E+000 atm-m³/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 6. 01 (KowWin est)Log Kaw used: 2. 582 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 3. 428Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2986Biowin2 (Non-Linear Model) : 0. 0543Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 3985 (weeks-months)Biowin4 (Primary Survey Model) : 3. 2951 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5407Biowin6 (MITI Non-Linear Model): 0. 5599Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 2058Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 1. 5231BioHC Half-Life (days) : 33. 3510Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 325 Pa (2. 44 mm Hg)Log Koa (Koawin est) : 3. 428Kp (particle/gas partition coef. (m³/ug)): Mackay model : 9. 22E-009 Octanol/air (Koa) model: 6. 58E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 33E-007 Mackay model : 7. 38E-007 Octanol/air (Koa) model: 5. 26E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 6. 6559 E-12 cm³/molecule-secHalf-Life = 1. 607 Days (12-hr day; 1. 5E6 OH/cm³)Half-Life = 19. 284 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 5. 35E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 2467Log Koc: 3. 392 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. 930 (BCF = 8503)log Kow used: 6. 01 (estimated)Volatilization from Water: Henry LC: 9. 35 atm-m³/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 332 hoursHalf-Life from Model Lake : 124 hours (5. 165 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 99. 95 percentTotal biodegradation: 0. 18 percentTotal sludge adsorption: 58. 66 percentTotal to Air: 41. 12 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 2. 19 38. 6 1000 Water 5. 73 900 1000 Soil 6. 69 1. 8e+003 1000 Sediment 85. 4 8. 1e+003 0 Persistence Time: 1. 2e+003 hr

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