

# [2,2,7,7-tetramethyloctane c12h26 structure](https://assignbuster.com/2277-tetramethyloctane-c12h26-structure/)

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):

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| --- |
| 1045 (estimated with error: 39)NIST Spectramainlib\_113585  |

## Retention Index (Linear):

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| 1038. 54 (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: 1 K/min; Start T: -30 C; End T: 240 C; CAS no: 1071314; Active phase: Ultra-1; 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 ri  |
| 1039. 44 (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: 2 K/min; Start T: -30 C; End T: 240 C; CAS no: 1071314; Active phase: Ultra-1; 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 ri  |
| 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: Ultra-1; 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 ri  |
| 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: 4 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.; Hartonen, K.; Reissell, A.; Vreuls, R.; Adahchour, M.; Hyotylainen, T., Comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry in 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 ri  |
| 1036. 7 (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: 2 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 ri  |
| 1036. 75 (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: 3 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 ri  |

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

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| --- | --- |
| 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  |

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| --- | --- |
| 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 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) = 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 OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 9. 35E+000 atm-m3/moleGroup Method: 1. 94E+001 atm-m3/moleHenrys 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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