

# [7-acetyl-6-ethyl-1,1,4,4-tetramethyltetralin c18h26o structure](https://assignbuster.com/7-acetyl-6-ethyl-1144-tetramethyltetralin-c18h26o-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 18 H 26 O  |
| Average mass  | 258. 398 Da  |
| Density  | 0. 9±0. 1 g/cm 3  |
| Boiling Point  | 361. 9±41. 0 °C at 760 mmHg  |
| Flash Point  | 152. 6±22. 6 °C  |
| Molar Refractivity  | 81. 3±0. 3 cm 3  |
| Polarizability  | 32. 2±0. 5 10 -24 cm 3  |
| Surface Tension  | 32. 3±3. 0 dyne/cm  |
| Molar Volume  | 277. 4±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Predicted – Mcule
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| 46. 5 °CJean-Claude Bradley Open Melting Point Dataset21003  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1997 (estimated with error: 57)NIST Spectramainlib\_161672, replib\_79559, replib\_261786  |
| 1790. 6 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 35 mm; Column length: 40 m; Column type: Capillary; Start T: 100 C; CAS no: 88299; Active phase: SE-30; Phase thickness: 0. 35 um; Data type: Kovats RI; Authors: Tudor, E., Temperature dependence of the retention index for perfumery compounds on a SE-30 glass capillary column. I. Linear equations, J. Chromatogr. A, 779, 1997, 287-297.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1788. 3 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 90 C; End T: 300 C; End time: 10 min; CAS no: 88299; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Osemwengie, L. I.; Steinberg, S., Closed-loop stripping analysis of synthetic musk compounds from fish tissues with measurement by gas chromatography-mass spectrometry with selected-ion monitoring, J. Chromatogr. A, 993, 2003, 1-15.)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:  | 361. 9±41. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 8 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 60. 8±3. 0 kJ/mol  |
| Flash Point:  | 152. 6±22. 6 °C  |
| Index of Refraction:  | 1. 498  |
| Molar Refractivity:  | 81. 3±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 2  |
| #Rule of 5 Violations:  | 1  |

|  |  |
| --- | --- |
| ACD/LogP:  | 6. 41  |
| ACD/LogD (pH 5. 5):  | 5. 75  |
| ACD/BCF (pH 5. 5):  | 13786. 66  |
| ACD/KOC (pH 5. 5):  | 31960. 45  |
| ACD/LogD (pH 7. 4):  | 5. 75  |
| ACD/BCF (pH 7. 4):  | 13786. 66  |
| ACD/KOC (pH 7. 4):  | 31960. 45  |
| Polar Surface Area:  | 17 Å 2  |
| Polarizability:  | 32. 2±0. 5 10 -24 cm 3  |
| Surface Tension:  | 32. 3±3. 0 dyne/cm  |
| Molar Volume:  | 277. 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) = 5. 87Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 329. 65 (Adapted Stein & Brown method)Melting Pt (deg C): 106. 95 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 000124 (Modified Grain method)Subcooled liquid VP: 0. 000789 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 2066log Kow used: 5. 87 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 20102 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Vinyl/Allyl KetonesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 57E-004 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 041E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 87 (KowWin est)Log Kaw used: -1. 979 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 849Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2635Biowin2 (Non-Linear Model) : 0. 0104Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 1814 (months )Biowin4 (Primary Survey Model) : 3. 1458 (weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3001Biowin6 (MITI Non-Linear Model): 0. 0974Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -1. 0628Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 105 Pa (0. 000789 mm Hg)Log Koa (Koawin est ): 7. 849Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 85E-005 Octanol/air (Koa) model: 1. 73E-005 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 00103 Mackay model : 0. 00228 Octanol/air (Koa) model: 0. 00139 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 253. 2385 E-12 cm3/molecule-secHalf-Life = 0. 042 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 507 HrsOzone Reaction: OVERALL Ozone Rate Constant = 14. 390500 E-17 cm3/molecule-secHalf-Life = 0. 080 Days (at 7E11 mol/cm3)Half-Life = 1. 911 HrsFraction sorbed to airborne particulates (phi): 0. 00165 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 5998Log Koc: 3. 778 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. 819 (BCF = 6590)log Kow used: 5. 87 (estimated)Volatilization from Water: Henry LC: 0. 000257 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 5. 303 hoursHalf-Life from Model Lake : 192. 6 hours (8. 026 days)Removal In Wastewater Treatment: Total removal: 91. 57 percentTotal biodegradation: 0. 76 percentTotal sludge adsorption: 90. 49 percentTotal to Air: 0. 32 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 013 0. 662 1000 Water 3. 13 1. 44e+003 1000 Soil 45. 9 2. 88e+003 1000 Sediment 51 1. 3e+004 0 Persistence Time: 3. 02e+003 hr

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