

7-acetyl-6-ethyl-  
1,1,4,4-  
tetramethyltetralin  
c<sub>18</sub>h<sub>26</sub>o structure



**ASSIGN  
BUSTER**

## Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_{18}H_{26}O$
Average mass	258.398 Da
Density	$0.9 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$361.9 \pm 41.0$ °C at 760 mmHg
Flash Point	$152.6 \pm 22.6$ °C
Molar Refractivity	$81.3 \pm 0.3 \text{ cm}^3$
Polarizability	$32.2 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	$32.3 \pm 3.0$ dyne/cm
Molar	$277.4 \pm 3.0 \text{ cm}^3$

Volume 3

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

- **Experimental Melting Point:**

46.5 °C

Claude Bradley

Open Melting

Point

Dataset21003

- Gas Chromatography

- **Retention Index (Kovats):**

1997 (estimated

with error:

57)NIST

Spectramainlib\_1

61672,

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 <sup>3</sup>
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 <sup>3</sup>
#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

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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 <sup>2</sup>
Polarizability:	32. 2±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	32. 3±3. 0 dyne/cm
Molar Volume:	277. 4±3. 0 cm <sup>3</sup>

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 KetonesHenry's Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 57E-004 atm-m<sup>3</sup>/moleGroup Method: IncompleteHenry's LC [VP/WSol estimate using EPI values]: 2. 041E-004 atm-m<sup>3</sup>/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

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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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- 1-Click Scaffold Hop