Unii:5f602cf6qf c10h18o structure

Contents

Molecular Formula	$C_{10}H_{18}O$
Average mass	154. 249 Da
Density	0. 9±0. 1 g/cm ^{3}
Boiling Point	225. 4±9. 0 °C at 760 mmHg
Flash Point	103. 3±0. 0 °C
Molar Refractivity	47. 4±0. 3 cm ^{3}
Polarizability	18. 8±0. 5 10^{-24} cm ^{3}
Surface Tension	31. 9±3. 0 dyne/cm
Molar	167. 3±3. 0

Volume cm^3

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

Retention Index (Kovats):

1230

(estimated

with error:

41)NIST

Spectramainl

ib_185271,

mainlib_2378

79,

mainlib_2162

2,

replib_92302

,

replib_5068,

replib_15192

5,

replib_21621

,

replib_18527

2

- **Retention Index (Linear):**

1288

(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: 2

K/min; Start

T: 70 C; End

T: 230 C;

CAS no:

13835751;

Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Song, H. S.; Sawamura, M.; Ito, T.; Kawashimo, K.; Ukeda, H., Quantitative determinatio n of characteric flavour of Citrus junos (yuzu) peel oil, Flavour Fragr. J., 15, 2000, 245-250.)NIST Spectranist ri

1924

(Program

type: Ramp;

Column cl…

(show

more)ass:

Standard

polar;

Column type:

Packed; CAS

no:

13835751;

Active phase:

DB-Wax;

Data type:

Linear RI;

Authors:

Rouseff, R.;

Smoot, J.;

Valim, F.;

Dreher, G.;

Mahattanata

wee, k.; Bell,

W.; Blaze, M.,

Flavor

Database,

2002.)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:	225. 4±9. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 0 mmHg at 25°C
Enthalpy of Vaporization:	53. 7±6. 0 kJ/mol
Flash Point:	103. 3±0. 0 °C
Index of Refraction:	1. 478
Molar Refractivity:	47. 4±0. 3 cm ^{3}
#H bond acceptors:	1
#H bond donors:	1
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0
ACD/LogP:	2. 89
ACD/LogD (pH 5. 5):	3. 02

ACD/BCF (pH 5. 5):	115. 16
ACD/KOC (pH 5. 5):	1040. 13
ACD/LogD (pH 7. 4):	3. 02
ACD/BCF (pH 7. 4):	115. 16
ACD/KOC (pH 7. 4):	1040. 13
Polar Surface Area:	20 Å ^{2}
Polarizability:	18. 8±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	31. 9±3. 0 dyne/cm
Molar Volume:	167. 3±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) = 3. 37Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 236. 58 (Adapted Stein & Brown method)Melting Pt (deg C): 10. 13 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00767 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 311. 7log Kow used: 3. 37 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1203. 3 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 58E-005 atm-m3/moleGroup Method: 3. 54E-006 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 994E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 37 (KowWin est)Log Kaw used: -3. 190 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 6. 560Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8328Biowin2 (Non-Linear Model) : 0. 8739Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model):

3. 0183 (weeks)Biowin4 (Primary Survey Model) : 3. 7546 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4918Biowin6 (MITI Non-Linear Model): 0. 5135Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2757Ready 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. 965 Pa (0. 00724 mm Hg)Log Koa (Koawin est): 6. 560Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 11E-006 Octanol/air (Koa) model: 8. 91E-007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000112 Mackay model : 0. 000249 Octanol/air (Koa) model: 7. 13E-005 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 101. 6199 E-12 cm3/molecule-secHalf-Life = 0. 105 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 263 HrsOzone Reaction: OVERALL Ozone Rate Constant = 43. 000000 E-17 cm3/molecule-secHalf-Life = 0. 027 Days (at 7E11 mol/cm3)Half-Life = 38. 378 MinReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 0. 00018 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 77. 35Log Koc: 1. 888 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 = 1. 894 (BCF = 78. 42)log Kow used: 3. 37 (estimated)Volatilization from Water: Henry LC: 3. 54E-006 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 206. 7 hours (8. 612 days)Half-Life from Model Lake : 2359 hours (98. 28 days)Removal In Wastewater Treatment: Total removal: 10. 57 percentTotal biodegradation: 0. 16 percentTotal sludge adsorption: 10. 22 percentTotal to Air: 0. 18 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0538 0. 51 1000 Water 24. 7 360 1000 Soil 74. 4 720 1000 Sediment 0. 844 3. 24e+003 0 Persistence Time: 459 hr

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