7,9-di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione c17h24o3 structure

ASSIGN BUSTER

Contents

Molecular Formula	$C_{17}H_{24}O_3$
Average mass	276. 371 Da
Density	1. 1±0. 1 g/cm ^{3}
Boiling Point	426. 3±45. 0 °C at 760 mmHg
Flash Point	187. 5±28. 8 °C
Molar Refractivity	78. 0±0. 4 cm ^{3}
Polarizability	30. 9±0. 5 10^{-24} cm ^{3}
Surface Tension	37. 2±5. 0 dyne/cm
Molar	258. 9±5. 0

Volume cm^3

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

Retention Index (Kovats):

2081

(estimated

with error:

89)NIST

Spectramainl

ib_279726,

replib_26413

8

Retention Index (Linear):

1929

(Program

type: Ramp;

Column cl...

(show

more)ass:

Semi-

standard

non-polar;

Column

diameter: 0.

25 mm;

Column

length: 60 m;

Column type:

Capillary;

Heat rate: 3

K/min; Start

T: 40 C; End

T: 310 C; End

time: 20 min;

Start time: 1

min; CAS no:

82304663;

Active phase:

HP-5MS;

Carrier gas:

He; Phase

thickness: 0.

25 um; Data

type: Linear

RI; Authors:

Lalel, H. J. D.;
Singh, Z.;
Chye Tan, S.,
Glycosidically
-bound
aroma
volatile
compounds
in the skin
and pulp of ‘
Kensington
Pride’ mango
fruit at
different
stages of
maturity,
Postharvest
Biol.
Technol., 29,
2003, 205-
218.)NIST
Spectranist ri

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

Density:	1. 1±0. 1 g/cm ^{3}
Boiling Point:	426. 3±45. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 0 mmHg at 25°C
Enthalpy of Vaporization:	68. 1±3. 0 kJ/mol
Flash Point:	187. 5±28. 8 °C
Index of Refraction:	1. 515
Molar Refractivity:	78. 0±0. 4 cm ^{3}
#H bond acceptors:	3
#H bond donors:	0
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0
ACD/LogP:	3. 08
ACD/LogD (pH 5. 5):	3. 48
ACD/BCF (pH 5. 5):	260. 29
ACD/KOC (pH 5. 5):	1864. 61
ACD/LogD (pH 7. 4):	3. 48

ACD/BCF (pH 7. 4):	260. 29
ACD/KOC (pH 7. 4):	1864. 61
Polar Surface Area:	43 Å ^{2}
Polarizability:	30. 9±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	37. 2±5. 0 dyne/cm
Molar Volume:	258. 9±5. 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. 55Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 384. 56 (Adapted Stein & Brown method)Melting Pt (deg C): 134. 94 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 54E-006 (Modified Grain method)Subcooled liquid VP: 1. 97E-005 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): 15. 5log Kow used: 3. 55 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3. 9542 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersVinyl/Allyl KetonesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 11E-007 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 613E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 55 (KowWin est)Log Kaw used: -5. 064 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 8. 614Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2452Biowin2 (Non-Linear Model) : 0. 0788Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 0698 (months)Biowin4 (Primary Survey Model) : 3. 1954 (weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6085Biowin6 (MITI Non-Linear Model): 0. 4183Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -1. 2512Ready 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. 00263 Pa (1. 97E-005 mm Hg)Log Koa (Koawin est): 8. 614Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 00114 Octanol/air (Koa) model: 0. 000101 Fraction sorbed to

airborne particulates (phi): Junge-Pankow model : 0. 0396 Mackay model : 0. 0837 Octanol/air (Koa) model: 0. 00801 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 62. 9660 E-12 cm3/molecule-secHalf-Life = 0. 170 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 2. 038 HrsOzone Reaction: OVERALL Ozone Rate Constant = 0. 350000 E-17 cm3/molecule-secHalf-Life = 3. 274 Days (at 7E11 mol/cm3)Half-Life = 78. 583 HrsFraction sorbed to airborne particulates (phi): 0. 0617 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 666. 1Log Koc: 2. 824 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 = 2. 037 (BCF = 108. 8)log Kow used: 3. 55 (estimated)Volatilization from Water: Henry LC: 2. 11E-007 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 4615 hours (192. 3 days)Half-Life from Model Lake : 5. 048E+004 hours (2103 days)Removal In Wastewater Treatment: Total removal: 14. 23 percentTotal biodegradation: 0. 19 percentTotal sludge adsorption: 14. 03 percentTotal to Air: 0. 01 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0989 3. 88 1000 Water 13. 9 1. 44e+003 1000 Soil 84. 7 2. 88e+003 1000 Sediment 1. 35 1. 3e+004 0 Persistence Time: 1. 68e+003 hr

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