

# [7,9-di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione c17h24o3 structure](https://assignbuster.com/79-di-tert-butyl-1-oxaspiro45deca-69-diene-28-dione-c17h24o3-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| 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 Volume | 258. 9±5. 0 cm 3 |

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

## Retention Index (Kovats):

|  |
| --- |
| 2081 (estimated with error: 89)NIST Spectramainlib\_279726, replib\_264138 |

## 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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