1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)disilaphosphane c9h27?3 structure

Contents

Molecular Formula	$C_9H_{27}?_3$
Average mass	250. 541 Da
Density	
Boiling Point	243. 5±0. 0 °C at 760 mmHg
Flash Point	87. 1±22. 6 °C
Molar Refractivity	
Polarizabilit y	
Surface Tension	

Molar

Volume

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

Experimental Melting Point:

24 °CAlfa

Aesar

24 °CJean-

Claude

Bradley

Open

Melting

Point

Dataset869

9

24 °CAlfa

Aesar30218

Experimental Boiling Point:

102-105 deg

C / 16 mm

(238. 1511-

242. 1397

°C / 760

mmHg)Alfa

Aesar

102-105 °C /

16 mm

(238. 1511-

242. 1397

°C / 760

mmHg)Alfa

Aesar30218

- **Experimental Gravity:**

  0. 863

  g/mLAlfa

  Aesar30218

- **Experimental Refraction Index:**

  1. 502Alfa

  Aesar30218

- Miscellaneous

- **Safety:**

17-

36/38Alfa

Aesar30218

4. 2Alfa

Aesar30218

7-17-26-

37Alfa

Aesar30218

DangerAlfa

Aesar30218

DANGER:

PYROPHORI

C, burns

skin and

eyesAlfa

Aesar30218

H250-H252-

H315-

H319Alfa

Aesar30218

P210-P222-

P280-

P305+P351

+P338-

P362-

P422aAlfa

Aesar30218

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

Density:	
Boiling Point:	243. 5±0. 0 °C at 760 mmHg
Vapour Pressure:	0. 1±0. 4 mmHg at 25°C
Enthalpy of Vaporization:	46. 1±3. 0 kJ/mol
Flash Point:	87. 1±22. 6 °C
Index of Refraction:	
Molar Refractivity:	
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0

ACD/LogP:	4. 82
ACD/LogD (pH 5. 5):	6. 15
ACD/BCF (pH 5. 5):	27992. 27
ACD/KOC (pH 5. 5):	53060. 93
ACD/LogD (pH 7. 4):	6. 15
ACD/BCF (pH 7. 4):	27992. 27
ACD/KOC (pH 7. 4):	53060. 93
Polar Surface Area:	14 Å ^{2}
Polarizability:	
Surface Tension:	
Molar Volume:	

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. 56Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 156. 18 (Adapted Stein & Brown method)Melting Pt (deg C): -58. 84 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 3. 01 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 4228log Kow used: 5. 56 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3. 9964e-005 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es)

found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 95E-002 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 347E+000 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 56 (KowWin est)Log Kaw used: -0. 098 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 5. 658Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6283Biowin2 (Non-Linear Model) : 0. 3661Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 6455 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4863 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 0295Biowin6 (MITI Non-Linear Model): 0. 0106Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 1199Ready 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): 365 Pa (2. 74 mm Hg)Log Koa (Koawin est): 5. 658Kp (particle/gas partition coef. (m3/ug)): Mackay model : 8. 21E-009 Octanol/air (Koa) model: 1. 12E-007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 97E-007 Mackay model : 6. 57E-007 Octanol/air (Koa) model: 8. 93E-006 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 1. 3464 E-12 cm3/molecule-secHalf-Life = 7. 944 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 95. 330 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 4. 77E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 2997Log Koc: 3. 477 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. 578 (BCF = 3785)log Kow used: 5. 56 (estimated)Volatilization from Water: Henry LC: 0. 0195 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 663 hoursHalf-Life from Model Lake : 150. 9 hours (6. 286 days)Removal In Wastewater Treatment: Total removal: 94. 15 percentTotal biodegradation: 0. 48 percentTotal sludge adsorption: 73. 12 percentTotal to Air: 20. 56 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 2. 5 191 1000 Water 5. 07 900 1000 Soil 56. 2 1. 8e+003 1000 Sediment 36. 3 8. 1e+003 0 Persistence Time: 1. 46e+003 hr

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