

# [1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)disilaphosphane c9h27?3 structure](https://assignbuster.com/111333-hexamethyl-2-trimethylsilyldisilaphosphane-c9h273-structure/)

Contents

* Safety:

|  |  |
| --- | --- |
| Molecular Formula  | C 9 H 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  |  |
| Polarizability  |  |
| 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 Dataset8699  |
| 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: PYROPHORIC, 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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