

# [1,1,1,3,5,5,5-heptamethyltrisiloxane c7h22o2si3 structure](https://assignbuster.com/1113555-heptamethyltrisiloxane-c7h22o2si3-structure/)

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* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula | C 7 H 22 O 2 Si 3 |
| Average mass | 222. 505 Da |
| Density |  |
| Boiling Point | 163. 8±23. 0 °C at 760 mmHg |
| Flash Point | 52. 8±22. 6 °C |
| Molar Refractivity |  |
| Polarizability |  |
| Surface Tension |  |
| Molar Volume |  |

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

## Experimental Boiling Point:

|  |
| --- |
| 142 °COxford University Chemical Safety Data (No longer updated)More details |
| 142 °CAlfa AesarH60586 |
| 141-142 °CSynQuest52912, 6183-1-02 |
| 141 °COakwood[S09300] |
| 141 °CLabNetworkLN00198439 |

## Experimental Flash Point:

|  |
| --- |
| 22 °COxford University Chemical Safety Data (No longer updated)More details |
| 22 °CAlfa Aesar |
| 22 °F (-5. 5556 °C)Alfa AesarH60586 |
| 27 °CSynQuest52912, 6183-1-02 |
| 27 °COakwood[S09300] |
| 22 °CLabNetworkLN00198439 |

## Experimental Gravity:

|  |
| --- |
| 0. 819 g/mLAlfa AesarH60586 |
| 0. 813 g/mLSynQuest6183-1-02 |
| 0. 8136 g/mLOakwood[S09300] |
| 0. 98 g/mLFluorochem |
| 0. 99 g/mLFluorochem |
| 0. 98 g/lFluorochemHMS-991, HMS-992, HMS-993 |
| 0. 99 g/lFluorochemHMS-991, HMS-992, HMS-993 |

## Experimental Refraction Index:

|  |
| --- |
| 1. 3815SynQuest52912, 6183-1-02 |

* Miscellaneous

## Appearance:

|  |
| --- |
| colourless liquidOxford University Chemical Safety Data (No longer updated)More details |

## Stability:

|  |
| --- |
| Stable. Flammable. Incompatible with strong oxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details |

## Safety:

|  |
| --- |
| 10-36/37/38Alfa AesarH60586 |
| 23-26-37-60Alfa AesarH60586 |
| 3Alfa AesarH60586 |
| DangerAlfa AesarH60586 |
| H225-H315-H319-H335Alfa AesarH60586 |
| IRRITANTMatrix Scientific097472 |
| P210-P261-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarH60586 |
| Safety glasses, adequate ventilation. Oxford University Chemical Safety Data (No longer updated)More details |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 743 (estimated with error: 89)NIST Spectramainlib\_104190 |

## Retention Index (Normal Alkane):

|  |
| --- |
| 842. 4 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2 m; Column type: Packed; CAS no: 1873887; Active phase: Lucopren G (silicone elastomer); Carrier gas: N2; Substrate: Celite 545 (0. 12-0. 15 mm); Data type: Normal alkane RI; Authors: Wurst, M.; Churacek, J., Analyse von organosiliciumverbindungen. VI. Retentionsindices der organosiliciumverbindungen bie der gaschromatographie, Collect. Czech. Chem. Commun., 36, 1971, 3497-3506.)NIST Spectranist ri |

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

|  |  |
| --- | --- |
| Density: |  |
| Boiling Point: | 163. 8±23. 0 °C at 760 mmHg |
| Vapour Pressure: | 2. 7±0. 3 mmHg at 25°C |
| Enthalpy of Vaporization: | 38. 4±3. 0 kJ/mol |
| Flash Point: | 52. 8±22. 6 °C |
| Index of Refraction: |  |
| Molar Refractivity: |  |
| #H bond acceptors: | 2 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 4 |
| #Rule of 5 Violations: | 1 |

|  |  |
| --- | --- |
| ACD/LogP: | 5. 32 |
| ACD/LogD (pH 5. 5): | 4. 45 |
| ACD/BCF (pH 5. 5): | 1428. 10 |
| ACD/KOC (pH 5. 5): | 6306. 32 |
| ACD/LogD (pH 7. 4): | 4. 45 |
| ACD/BCF (pH 7. 4): | 1428. 10 |
| ACD/KOC (pH 7. 4): | 6306. 32 |
| Polar Surface Area: | 18 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) = 7. 78Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): -7. 34 (Adapted Stein & Brown method)Melting Pt (deg C): -36. 32 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 38E+003 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 0005123log Kow used: 7. 78 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 9. 6628e-007 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : IncompleteGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 4. 343E+005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Can Not Estimate (can not calculate HenryLC)Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : -0. 6459Biowin2 (Non-Linear Model) : 0. 0000Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 1. 2226 (recalcitrant)Biowin4 (Primary Survey Model) : 2. 4526 (weeks-months)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5235Biowin6 (MITI Non-Linear Model): 0. 2488Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -1. 5035Ready 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): 3. 09E+005 Pa (2. 32E+003 mm Hg)Log Koa (): not availableKp (particle/gas partition coef. (m3/ug)): Mackay model : 9. 7E-012 Octanol/air (Koa) model: not availableFraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 5E-010 Mackay model : 7. 76E-010 Octanol/air (Koa) model: not availableAtmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 0000 E-12 cm3/molecule-secHalf-Life = -------Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 5. 63E-010 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 2167Log Koc: 3. 336 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. 748 (BCF = 5599)log Kow used: 7. 78 (estimated)Volatilization from Water: Henry LC: 4. 34E+005 atm-m3/mole (calculated from VP/WS)Half-Life from Model River: 1. 522 hoursHalf-Life from Model Lake : 141. 7 hours (5. 903 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 100. 00 percentTotal biodegradation: 0. 18 percentTotal sludge adsorption: 59. 87 percentTotal to Air: 39. 95 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 1. 05 1e+005 1000 Water 1. 25 4. 32e+003 1000 Soil 0. 0111 8. 64e+003 1000 Sediment 97. 7 3. 89e+004 0 Persistence Time: 6. 38e+003 hr

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