# 1,1,1,3,5,5,5-heptamethyltrisiloxane c7h22o2si3 structure

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| | |
|---|---|
| Molecular Formula | $C_7H_{22}O_2Si_3$ |
| 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

°CLabNetworkLN00198

439

- **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

  °CLabNetworkLN00198

439

- **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

  organosiliciumverbindu

  ngen. VI.

  Retentionsindices der

organosiliciumverbindu

ngen 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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