

# [Tetraethyl orthosilicate c8h20o4si structure](https://assignbuster.com/tetraethyl-orthosilicate-c8h20o4si-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 8 H 20 O 4 Si  |
| Average mass  | 208. 327 Da  |
| Density  | 0. 9±0. 1 g/cm 3  |
| Boiling Point  | 165. 5±0. 0 °C at 760 mmHg  |
| Flash Point  | 46. 7±0. 0 °C  |
| Molar Refractivity  | 54. 8±0. 3 cm 3  |
| Polarizability  | 21. 7±0. 5 10 -24 cm 3  |
| Surface Tension  | 23. 5±3. 0 dyne/cm  |
| Molar Volume  | 221. 8±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -85 °CAlfa Aesar  |
| -86 °COxford University Chemical Safety Data (No longer updated)More details  |
| -86 °CJean-Claude Bradley Open Melting Point Dataset16140  |
| -82. 5 °CJean-Claude Bradley Open Melting Point Dataset21205  |
| -85 °CJean-Claude Bradley Open Melting Point Dataset8480  |
| -85 °CAlfa Aesar14082, 22967, 40251, A14965  |
| 285 °CBiosynthQ-201810  |
| -77 °CLabNetworkLN00175733  |

## Experimental Boiling Point:

|  |
| --- |
| 168 °CAlfa Aesar  |
| 169 °COxford University Chemical Safety Data (No longer updated)More details  |
| 168 °CAlfa Aesar14082, 22967, 40251, A14965  |
| 168 °CSynQuest6183-1-42  |
| 169 °COakwoodS15425  |
| 168 °C (Literature)LabNetworkLN00175733  |

## Experimental Flash Point:

|  |
| --- |
| 46 °CAlfa Aesar  |
| 39 °COxford University Chemical Safety Data (No longer updated)More details  |
| 46 °CAlfa Aesar  |
| 46 °F (7. 7778 °C)Alfa Aesar14082, 22967, 40251, A14965  |
| 48 °CSynQuest6183-1-42  |
| 46 °COakwoodS15425  |
| 54 °CLabNetworkLN00175733  |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLMerck Millipore1940  |
| 20 g/lMerck Millipore1940, 800658  |
| 0. 934 g/mLAlfa Aesar14082, 22967, 40251, A14965  |
| 0. 93 g/mLMatrix Scientific076014  |
| 0. 934 g/mLSynQuest6183-1-42  |
| 0. 9335 g/mLOakwoodS15425  |
| 0. 933 g/mLFluorochem  |
| 0. 933 g/lFluorochemS15425  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 382Alfa AesarA14965, 40251, 22967, 14082  |

* Miscellaneous

## Appearance:

|  |
| --- |
| colourless liquid with an alcohol-like odourOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

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

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 6270 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 10-20-36/37Alfa Aesar14082, 22967, 40251, A14965  |
| 2Alfa Aesar14082, 22967, 40251, A14965  |
| 3Alfa Aesar14082, 22967, 40251, A14965  |
| DANGER: FLAMMABLE, causes narcosis, irritationAlfa Aesar14082, 22967, 40251  |
| DANGER: FLAMMABLE, irritates skin, eyes, lungsAlfa AesarA14965  |
| Flammable/Harmful/Moisture Sensitive/Store under ArgonSynQuest6183-1-42  |
| GHS07BiosynthQ-201810  |
| H226-H332-H319-H335Alfa Aesar14082, 22967, 40251, A14965  |
| H315; H319; H335BiosynthQ-201810  |
| IRRITANTMatrix Scientific076014  |
| P210-P261-P303+P361+P353-P305+P351+P338-P405-P501aAlfa Aesar14082, 22967, 40251, A14965  |
| P261; P280; P302+P352; P304+P340; P305+P351+P338; P312BiosynthQ-201810  |
| R10, R20, R36/37/38SynQuest6183-1-42  |
| S9, S16, S23, S24/25, S26, S36/37/39, S38, S45SynQuest6183-1-42  |
| Safety glasses, adequate ventilation. Vapour is much heavierthan air, and precautions should be taken to prevent the vapourflowing to a source of ignition. Oxford University Chemical Safety Data (No longer updated)More details  |
| WarningAlfa Aesar14082, 22967, 40251, A14965  |
| WarningBiosynthQ-201810  |
| WARNING: Irritates skin and eyes, harmful if swallowedAlfa AesarA14965  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1030 (estimated with error: 89)NIST Spectramainlib\_9586, replib\_158593, replib\_233769  |
| 850 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1 m; Column type: Packed; Start T: 150 C; CAS no: 78104; Active phase: Apiezon L; Carrier gas: Ar; Data type: Kovats RI; Authors: Kreshkov, A. P.; Kirichenko, E. A.; Markov, B. A., Retention indices of alkoxychlorosilanes, Zh. Anal. Khim., 30(2), 1975, 286-289, In original 345-348.)NIST Spectranist ri  |
| 869 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 1 m; Column type: Packed; Start T: 100 C; CAS no: 78104; Active phase: Apiezon L; Carrier gas: Ar; Data type: Kovats RI; Authors: Kreshkov, A. P.; Kirichenko, E. A.; Markov, B. A., Retention indices of alkoxychlorosilanes, Zh. Anal. Khim., 30(2), 1975, 286-289, In original 345-348.)NIST Spectranist ri  |
| 847 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; CAS no: 78104; Active phase: Apiezon L; Data type: Kovats RI; Authors: Peetre, I.-B., Gas chromatographic investigation of organometallic compounds and their carbon analogues. II. Improved method for calculating retention indices of tetraalkoxysilanes, J. Chromatogr., 88, 1974, 311-321.)NIST Spectranist ri  |
| 851. 2 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 160 C; CAS no: 78104; Active phase: Apiezon L; Data type: Kovats RI; Authors: Peetre, I.-B., Gas chromatographic investigation of organometallic compounds and their carbon analogues. II. Improved method for calculating retention indices of tetraalkoxysilanes, J. Chromatogr., 88, 1974, 311-321.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 850 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 160 C; CAS no: 78104; Active phase: Apieson M; Substrate: Chromosorb G AW DMCS (80-100 mesh); Data type: Normal alkane RI; Authors: Ellren, O.; Peetre, I. B.; Smith, B. E. F., Gas chromatographic investigation of organometallic compounds and their carbon analogues. V. Use of refractive index in conjunction with Kovats retention index for the identification of organosilicon compounds, J. Chromatogr., 93, 1974, 383-392.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 0. 9±0. 1 g/cm 3  |
| Boiling Point:  | 165. 5±0. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 2. 5±0. 3 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 38. 5±3. 0 kJ/mol  |
| Flash Point:  | 46. 7±0. 0 °C  |
| Index of Refraction:  | 1. 409  |
| Molar Refractivity:  | 54. 8±0. 3 cm 3  |
| #H bond acceptors:  | 4  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 8  |
| #Rule of 5 Violations:  | 1  |

|  |  |
| --- | --- |
| ACD/LogP:  | 5. 10  |
| ACD/LogD (pH 5. 5):  | 1. 77  |
| ACD/BCF (pH 5. 5):  | 13. 05  |
| ACD/KOC (pH 5. 5):  | 218. 81  |
| ACD/LogD (pH 7. 4):  | 1. 77  |
| ACD/BCF (pH 7. 4):  | 13. 05  |
| ACD/KOC (pH 7. 4):  | 218. 81  |
| Polar Surface Area:  | 37 Å 2  |
| Polarizability:  | 21. 7±0. 5 10 -24 cm 3  |
| Surface Tension:  | 23. 5±3. 0 dyne/cm  |
| Molar Volume:  | 221. 8±3. 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) = 0. 04Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 208. 30 (Adapted Stein & Brown method)Melting Pt (deg C): 5. 75 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 65 (Mean VP of Antoine & Grain methods)MP (exp database): -82. 5 deg CBP (exp database): 168. 8 deg CVP (exp database): 1. 88E+00 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 3. 691e+004log Kow used: 0. 04 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Silanes (alkoxy)Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 97E-005 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 225E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 04 (KowWin est)Log Kaw used: -3. 094 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 3. 134Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6484Biowin2 (Non-Linear Model) : 0. 5126Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7388 (weeks-months)Biowin4 (Primary Survey Model) : 3. 5472 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2917Biowin6 (MITI Non-Linear Model): 0. 1554Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 6218Ready 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): 251 Pa (1. 88 mm Hg)Log Koa (Koawin est ): 3. 134Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 2E-008 Octanol/air (Koa) model: 3. 34E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 4. 32E-007 Mackay model : 9. 57E-007 Octanol/air (Koa) model: 2. 67E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 24. 6936 E-12 cm3/molecule-secHalf-Life = 0. 433 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 5. 198 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 6. 95E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 8766Log Koc: 3. 943 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 = 0. 500 (BCF = 3. 162)log Kow used: 0. 04 (estimated)Volatilization from Water: Henry LC: 1. 97E-005 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 44. 37 hours (1. 849 days)Half-Life from Model Lake : 605. 1 hours (25. 21 days)Removal In Wastewater Treatment: Total removal: 2. 92 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 74 percentTotal to Air: 1. 08 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 1. 28 10. 4 1000 Water 54. 5 900 1000 Soil 44. 1 1. 8e+003 1000 Sediment 0. 106 8. 1e+003 0 Persistence Time: 472 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop