Tetraethyl orthosilicate c8h20o4si structure

Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_8H_{20}O_4Si$
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

°CLabNetworkLN00175

733

- **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)LabNetwork

LN00175733

- **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

  °CLabNetworkLN00175

  733

- **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  colourless liquid with an alcohol-like odourOxford University Chemical Safety Data (No longer updated)More details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 Oxford University Chemical Safety Data (No longer updated)More details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  ORL-RAT LD50 6270 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details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,

R36/37/38SynQuest618

3-1-42

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

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- 1-Click Docking
- 1-Click Scaffold Hop