Trifluoromethanesulfonic anhydride c2f6o5s2 structure

Contents

- Retention Index (Kovats):

Molecular Formula	$C_2F_6O_5S_2$
Average mass	282. 139 Da
Density	2. 0±0. 1 g/cm ^{3}
Boiling Point	82. 6±0. 0 °C at 760 mmHg
Flash Point	-0. 6±25. 9 °C
Molar Refractivity	31. 4±0. 4 cm ^{3}
Polarizability	12. 5±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	34. 1±3. 0 dyne/cm
Molar Volume	142. 8±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite

- Predicted – ChemAxon
- Experimental Physico-chemical Properties

Experimental Melting Point:

-80 °CSynQuest

-80 °CAlfa Aesar

-80 °CJean-Claude

Bradley Open Melting

Point Dataset8636

-80 °CAlfa

AesarA11767

-80 °CSynQuest26910,

6164-2-13

80 °CBiosynthQ-

101271

-80

°CLabNetworkLN00008

016

Experimental Boiling Point:

81-83 °CAlfa Aesar

81-83 °CAlfa AesarA11767

83-84 °CSynQuest26910,

6164-2-13

81-83 °COakwood[007526]

81 °CBiosynthQ-101271

81-83

°CLabNetworkLN00008016

- **Experimental Vapor Pressure:**

8 mmHgSynQuest

8 °CSynQuest26910

8 mmHgSynQuest26910,

6164-2-13

- **Experimental Flash Point:**

83 °CBiosynthQ-

101271

- **Experimental Gravity:**

20 g/mLMerck Millipore2615

20 g/lMerck Millipore2615,

818043

1. 677 g/mLBiosynthQ-

101271

20 g/mLSynQuest6164-2-13

1. 72 g/mLAlfa AesarA11767

1. 677 g/mLSynQuest6164-2-

13

1. 677

g/mLOakwood[007526]

1. 677 g/mLFluorochem

83 g/mLBiosynthQ-101271

1. 677 g/lFluorochem007526

- **Experimental Refraction Index:**

  1. 321Alfa AesarA11767

  1. 3212SynQuest26910,

  6164-2-13

- Miscellaneous

- **Safety:**

  14-34Alfa AesarA11767

  8Alfa AesarA11767

  8-26-30-36/37/39-45-

  60Alfa AesarA11767

  Corrosive/Harmful/

  Moisture

  Sensitive/Store under

  ArgonSynQuest26910,

  6164-2-13

  DangerAlfa

  AesarA11767

  DangerBiosynthQ-

  101271

  DANGER: CORROSIVE,

  burns skin, eyes, and

  lungsAlfa AesarA11767

  DANGER: CORROSIVE,

  WATER REACTIVE,

  burns skin and eyes.

Alfa AesarA11767

GHS05;

GHS07BiosynthQ-

101271

H302; H314BiosynthQ-

101271

H314-EUH014Alfa

AesarA11767

P260-

P303+P361+P353-

P305+P351+P338-

P301+P330+P331-

P405-P501aAlfa

AesarA11767

P280;

P305+P351+P338;

P310BiosynthQ-101271

R14, R21/22, R34,

R36/37/38SynQuest269

10

R14, R21/22, R35,

R36/37/38SynQuest616

4-2-13

S3/7, S23, S24/25, S26,

S36/37/39, S43,

S45SynQuest26910

S7/8, S20/21, S23,

S24/25, S26, S27/28,

S36/37/39, S43, S45,

S46,

S49SynQuest6164-2-13

- Gas Chromatography

- **Retention Index (Kovats):**

  978 (estimated with

  error: 89)NIST

  Spectramainlib_235631

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

Density:	2. 0±0. 1 g/cm ^{3}
Boiling Point:	82. 6±0. 0 °C at 760 mmHg
Vapour Pressure:	86. 8±0. 1 mmHg at 25°C

Enthalpy of Vaporization:	31. 0±3. 0 kJ/mol
Flash Point:	-0. 6±25. 9 °C
Index of Refraction:	1. 359
Molar Refractivity:	31. 4±0. 4 cm^3
#H bond acceptors:	5
#H bond donors:	0
#Freely Rotating Bonds:	4
#Rule of 5 Violations:	0
ACD/LogP:	2. 12
ACD/LogD (pH 5. 5):	2. 87
ACD/BCF (pH 5. 5):	89. 10
ACD/KOC (pH 5. 5):	865. 64
ACD/LogD (pH 7. 4):	2. 87
ACD/BCF (pH 7. 4):	89. 10
ACD/KOC (pH 7. 4):	865. 64
Polar Surface Area:	94 $Å^2$

Polarizability:	12. 5±0. 5 10^{-24} cm^3
Surface Tension:	34. 1±3. 0 dyne/cm
Molar Volume:	142. 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) = 3. 66Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 273. 79 (Adapted Stein & Brown method)Melting Pt (deg C): 77. 09 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00248 (Modified Grain method)Subcooled liquid VP: 0. 00776 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 11. 6log Kow used: 3. 66 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 445. 03 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 17E-006 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 7. 937E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 66 (KowWin est)Log Kaw used: -4. 320 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 980Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : -0. 4276Biowin2 (Non-Linear Model) : 0. 0000Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 1. 5498 (recalcitrant)Biowin4 (Primary Survey Model) : 2. 8919 (weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 0229Biowin6 (MITI Non-Linear Model): 0. 0000Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8361Ready 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): 1. 03 Pa (0. 00776 mm Hg)Log Koa (Koawin est): 7. 980Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 9E-006 Octanol/air (Koa) model: 2. 34E-005 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000105 Mackay model : 0. 000232 Octanol/air (Koa) model: 0. 00187 Atmospheric 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): 0. 000168 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 133Log Koc: 2. 124 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 = 2. 121 (BCF = 132)log Kow used: 3. 66 (estimated)Volatilization from Water: Henry

LC: 1. 17E-006 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 842. 2 hours (35. 09 days)Half-Life from Model Lake : 9329 hours (388. 7 days)Removal In Wastewater Treatment: Total removal: 17. 26 percentTotal biodegradation: 0. 22 percentTotal sludge adsorption: 16. 99 percentTotal to Air: 0. 06 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 549 1e+005 1000 Water 6. 57 4. 32e+003 1000 Soil 91. 8 8. 64e+003 1000 Sediment 1. 12 3. 89e+004 0 Persistence Time: 4. 87e+003 hr