

# [Trifluoromethanesulfonic anhydride c2f6o5s2 structure](https://assignbuster.com/trifluoromethanesulfonic-anhydride-c2f6o5s2-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 2 F 6 O 5 S 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 °CLabNetworkLN00008016  |

## 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, R36/37/38SynQuest26910  |
| R14, R21/22, R35, R36/37/38SynQuest6164-2-13  |
| 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