

# [Chlorotrifluoroethene c2clf3 structure](https://assignbuster.com/chlorotrifluoroethene-c2clf3-structure/)

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* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 2 ClF 3  |
| Average mass  | 116. 470 Da  |
| Density  | 1. 4±0. 1 g/cm 3  |
| Boiling Point  | -23. 5±30. 0 °C at 760 mmHg  |
| Flash Point  | -43. 1±16. 5 °C  |
| Molar Refractivity  | 16. 4±0. 3 cm 3  |
| Polarizability  | 6. 5±0. 5 10 -24 cm 3  |
| Surface Tension  | 13. 5±3. 0 dyne/cm  |
| Molar Volume  | 82. 5±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -158. 2 °CSynQuest  |
| -129 °CSynQuest  |
| -158 °CJean-Claude Bradley Open Melting Point Dataset21157  |
| -129 °CSynQuest22483, 55845, 80717, 6734, 1100-6-33, 1100-6-42, 1100-6-45  |
| -158. 2 °CSynQuest22483, 55845, 80717, 6734, 1300-6-01  |

## Experimental Boiling Point:

|  |
| --- |
| -28 °CManchester Organics[N24662]  |
| 132 °CSynQuest1100-6-33, 1100-6-42, 1100-6-45  |
| -27 °CSynQuest22483, 55845, 80717, 6734, 1300-6-01  |

## Experimental Vapor Pressure:

|  |
| --- |
| 70 mmHgSynQuest  |
| 70 °CSynQuest22483, 55845, 80717, 6734  |
| 10 mmHgSynQuest1100-6-33, 1100-6-42, 1100-6-45  |
| 70 mmHgSynQuest22483, 55845, 80717, 6734, 1300-6-01  |

## Experimental Flash Point:

## Experimental Gravity:

|  |
| --- |
| 37. 8 g/mLSynQuest1100-6-33, 1100-6-42, 1100-6-45  |
| 20 g/mLSynQuest1300-6-01  |
| 1. 71 g/mLSynQuest1100-6-33, 1100-6-42, 1100-6-45  |
| 1. 305 g/mLSynQuest1300-6-01  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 383SynQuest22483, 55845, 80717, 6734, 1100-6-33, 1100-6-42, 1100-6-45  |

* Miscellaneous

## Safety:

|  |
| --- |
| Extremely Flammable/ToxicSynQuest22483, 55845, 1300-6-01, 6734, 80717  |
| IrritantSynQuest1100-6-33, 22483, 1100-6-42, 55845, 6734, 1100-6-45, 80717  |
| R12, R23/25, R36/37/38SynQuest22483, 55845, 1300-6-01, 6734, 80717  |
| R36/37/38SynQuest1100-6-33, 22483, 1100-6-42, 55845, 6734, 1100-6-45, 80717  |
| S16, S23, S24/25, S36/37, S38, S45SynQuest22483, 55845, 1300-6-01, 6734, 80717  |
| S23, S24/25, S36/37/39, S45SynQuest1100-6-33, 22483, 1100-6-42, 55845, 6734, 1100-6-45, 80717  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 277 (estimated with error: 89)NIST Spectramainlib\_1996, replib\_20387  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 294 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 79389; Active phase: Porapack Q; Data type: Normal alkane RI; Authors: Zenkevich, I. G.; Rodin, A. A., Gas chromatographic identification of some volatile toxic fluorine containing compounds by precalculated retention indices, J. Ecol. Chem. (Rus.), 13(1), 2004, 22-28.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 1. 4±0. 1 g/cm 3  |
| Boiling Point:  | -23. 5±30. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 3938. 5±0. 0 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 22. 0±3. 0 kJ/mol  |
| Flash Point:  | -43. 1±16. 5 °C  |
| Index of Refraction:  | 1. 321  |
| Molar Refractivity:  | 16. 4±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 2. 16  |
| ACD/LogD (pH 5. 5):  | 2. 02  |
| ACD/BCF (pH 5. 5):  | 20. 22  |
| ACD/KOC (pH 5. 5):  | 299. 43  |
| ACD/LogD (pH 7. 4):  | 2. 02  |
| ACD/BCF (pH 7. 4):  | 20. 22  |
| ACD/KOC (pH 7. 4):  | 299. 43  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 6. 5±0. 5 10 -24 cm 3  |
| Surface Tension:  | 13. 5±3. 0 dyne/cm  |
| Molar Volume:  | 82. 5±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) = 1. 65Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 7. 53 (Adapted Stein & Brown method)Melting Pt (deg C): -135. 72 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 4. 19E+003 (Mean VP of Antoine & Grain methods)MP (exp database): -158 deg CBP (exp database): -27. 8 deg CVP (exp database): 4. 59E+03 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 4013log Kow used: 1. 65 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 6789 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Vinyl/Allyl HalidesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 3. 11E-001 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 902E-002 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 65 (KowWin est)Log Kaw used: 1. 104 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 0. 546Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5807Biowin2 (Non-Linear Model) : 0. 3780Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7686 (weeks )Biowin4 (Primary Survey Model) : 3. 5791 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4189Biowin6 (MITI Non-Linear Model): 0. 0000Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8214Ready 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): 6. 12E+005 Pa (4. 59E+003 mm Hg)Log Koa (Koawin est ): 0. 546Kp (particle/gas partition coef. (m3/ug)): Mackay model : 4. 9E-012 Octanol/air (Koa) model: 8. 63E-013 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 77E-010 Mackay model : 3. 92E-010 Octanol/air (Koa) model: 6. 9E-011 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 2139 E-12 cm3/molecule-secHalf-Life = 49. 998 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: OVERALL Ozone Rate Constant = 0. 001602 E-17 cm3/molecule-secHalf-Life = 715. 534 Days (at 7E11 mol/cm3)Fraction sorbed to airborne particulates (phi): 2. 85E-010 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 106. 8Log Koc: 2. 029 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. 572 (BCF = 3. 733)log Kow used: 1. 65 (estimated)Volatilization from Water: Henry LC: 0. 311 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 103 hoursHalf-Life from Model Lake : 102. 5 hours (4. 272 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 99. 18 percentTotal biodegradation: 0. 02 percentTotal sludge adsorption: 0. 36 percentTotal to Air: 98. 79 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 31. 2 36. 6 1000 Water 67. 7 360 1000 Soil 0. 95 720 1000 Sediment 0. 176 3. 24e+003 0 Persistence Time: 90. 8 hr

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