Chlorotrifluoroethene c2clf3 structure

ASSIGN BUSTER

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Molecular Formula	C_2ClF_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

  mmHgSynQuest11

  00-6-33, 1100-6-

  42, 1100-6-45

  70

  mmHgSynQuest22

  483, 55845,

  80717, 6734,

  1300-6-01

- **Experimental Flash Point:**
- **Experimental Gravity:**

  37. 8

  g/mLSynQuest110

  0-6-33, 1100-6-42,

1100-6-45

20

g/mLSynQuest130

0-6-01

1. 71

g/mLSynQuest110

0-6-33, 1100-6-42,

1100-6-45

1. 305

g/mLSynQuest130

0-6-01

- **Experimental Refraction Index:**

  1.

  383SynQuest2248

  3, 55845, 80717,

  6734, 1100-6-33,

  1100-6-42, 1100-6-

  45

- Miscellaneous

  - **Safety:**

    Extremely

    Flammable/ToxicSy

nQuest22483,

55845, 1300-6-01,

6734, 80717

IrritantSynQuest11

00-6-33, 22483,

1100-6-42, 55845,

6734, 1100-6-45,

80717

R12, R23/25,

R36/37/38SynQues

t22483, 55845,

1300-6-01, 6734,

80717

R36/37/38SynQues

t1100-6-33, 22483,

1100-6-42, 55845,

6734, 1100-6-45,

80717

S16, S23, S24/25,

S36/37, S38,

S45SynQuest2248

3, 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_19

    96, 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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