Unii:b9mnd2bu7k c2hcl3f2 structure

Contents

Molecular Formula	$C_2HCl_3F_2$
Average mass	169. 385 Da
Density	1. 6±0. 1 g/cm ^{3}
Boiling Point	77. 9±8. 0 °C at 760 mmHg
Flash Point	-2. 5±11. 9 °C
Molar Refractivity	26. 1±0. 3 cm ^{3}
Polarizability	10. 4±0. 5 10^{-24} cm ^{3}
Surface Tension	24. 7±3. 0 dyne/cm
Molar Volume	107. 0±3. 0 cm ^{3}

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

Experimental Melting Point:

-173

°CSynQuest

-173 °CMatrix

Scientific

-173 °CMatrix

Scientific00917

6

-173

°CSynQuest173

82, 1100-7-13

Experimental Boiling Point:

72 °CMatrix Scientific

72 °CMatrix

Scientific009176

72 °CSynQuest17382,

1100-7-13

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

20

g/mLSynQuest1

100-7-13

1. 571

g/mLMatrix

Scientific00917

6

1. 571

g/mLSynQuest1

100-7-13

- Predicted Physico-chemical Properties
  - **Predicted Melting Point:**

-173 °CMatrix

Scientific009176

- Miscellaneous
  - **Safety:**

OZONE

DEPLETERMatri

x

Scientific00917

6

- Gas Chromatography

  - **Retention Index (Normal Alkane):**

    615 (Program

    type: Ramp;

    Column cl…

    (show

    more)ass: Semi-

    standard non-

    polar; Column

    length: 2 m;

    Column type:

    Packed; Heat

    rate: 5 K/min;

    Start T: 50 C;

    End T: 220 C;

    End time: 0

    min; Start time:

    0 min; CAS no:

    354154; Active

    phase:

    Porapack Q;

    Carrier gas:

Nitrogen; Data type: Normal alkane RI; Authors: Zenkevich, I. G.; Konukhova, S. V., Gas Chromatographic Identification of Ecologically Safe Freones, Vestn. of St. Petersburg Univ. (Rus.), , 1992, 66-70, In original 66-70.)NIST Spectranist ri

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

Density:	1. 6±0. 1 g/cm ^{3}
Boiling Point:	77. 9±8. 0 °C at 760 mmHg
Vapour Pressure:	104. 6±0. 1 mmHg at 25°C

Enthalpy of Vaporization:	30. 6±3. 0 kJ/mol
Flash Point:	-2. 5±11. 9 °C
Index of Refraction:	1. 403
Molar Refractivity:	26. 1±0. 3 cm^3
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	1
#Rule of 5 Violations:	0
ACD/LogP:	2. 36
ACD/LogD (pH 5. 5):	2. 47
ACD/BCF (pH 5. 5):	44. 80
ACD/KOC (pH 5. 5):	529. 19
ACD/LogD (pH 7. 4):	2. 47
ACD/BCF (pH 7. 4):	44. 80
ACD/KOC (pH 7. 4):	529. 19

Polar Surface Area:	0 Å ^{2}
Polarizability:	10. 4±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	24. 7±3. 0 dyne/cm
Molar Volume:	107. 0±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) = 2. 49Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 69. 10 (Adapted Stein & Brown method)Melting Pt (deg C): -77. 91 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 119 (Mean VP of Antoine & Grain methods)BP (exp database): 72. 5 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 84. 29log Kow used: 2. 49 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 525. 21 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 69E-002 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 147E-001 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 49 (KowWin est)Log Kaw used: -0. 161 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 651Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 1488Biowin2 (Non-Linear Model) : 0. 0013Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 0932 (months)Biowin4 (Primary Survey Model) : 3. 1481 (weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2632Biowin6 (MITI Non-Linear Model): 0. 0000Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2920Ready 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. 55E+004 Pa (116 mm Hg)Log Koa (Koawin est): 2. 651Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 94E-010 Octanol/air (Koa) model: 1. 1E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 7. 01E-009 Mackay model : 1. 55E-008 Octanol/air (Koa) model: 8. 79E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 0030 E-12 cm3/molecule-secHalf-Life = 3507. 963 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 1. 13E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 154. 4Log Koc: 2. 189 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 7. 736E+001 L/mol-secKb Half-Life at pH 8: 2. 489 hours Kb Half-Life at pH 7: 1. 037 days Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 1. 215 (BCF = 16. 41)log Kow used: 2. 49

(estimated)Volatilization from Water: Henry LC: 0. 0169 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 373 hoursHalf-Life from Model Lake : 124. 1 hours (5. 171 days)Removal In Wastewater Treatment: Total removal: 86. 90 percentTotal biodegradation: 0. 03 percentTotal sludge adsorption: 1. 23 percentTotal to Air: 85. 64 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 45. 9 1. 71e+004 1000 Water 45 1. 44e+003 1000 Soil 8. 81 2. 88e+003 1000 Sediment 0. 378 1. 3e+004 0 Persistence Time: 189 hr

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