

# [Unii:b9mnd2bu7k c2hcl3f2 structure](https://assignbuster.com/uniib9mnd2bu7k-c2hcl3f2-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 2 HCl 3 F 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 Scientific009176  |
| -173 °CSynQuest17382, 1100-7-13  |

## Experimental Boiling Point:

|  |
| --- |
| 72 °CMatrix Scientific  |
| 72 °CMatrix Scientific009176  |
| 72 °CSynQuest17382, 1100-7-13  |

## Experimental Flash Point:

## Experimental Gravity:

|  |
| --- |
| 20 g/mLSynQuest1100-7-13  |
| 1. 571 g/mLMatrix Scientific009176  |
| 1. 571 g/mLSynQuest1100-7-13  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| -173 °CMatrix Scientific009176  |

* Miscellaneous

## Safety:

|  |
| --- |
| OZONE DEPLETERMatrix Scientific009176  |

* 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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