

# [1,2-diiodoperfluoroethane c2f4i2 structure](https://assignbuster.com/12-diiodoperfluoroethane-c2f4i2-structure/)

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* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 2 F 4 I 2  |
| Average mass  | 353. 824 Da  |
| Density  | 2. 9±0. 1 g/cm 3  |
| Boiling Point  | 111. 0±8. 0 °C at 760 mmHg  |
| Flash Point  | 36. 0±5. 6 °C  |
| Molar Refractivity  | 37. 8±0. 3 cm 3  |
| Polarizability  | 15. 0±0. 5 10 -24 cm 3  |
| Surface Tension  | 32. 0±3. 0 dyne/cm  |
| Molar Volume  | 121. 1±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -21 °CSynQuest  |
| -21 °CAlfa Aesar  |
| -21 °CAlfa AesarA10954  |
| -21 °CSynQuest9195, 1100-J-03  |

## Experimental Boiling Point:

|  |
| --- |
| 112-113 °CAlfa Aesar  |
| 112-113 °CAlfa AesarA10954  |
| 112-113 °CSynQuest9195, 1100-J-03  |

## Experimental Flash Point:

## Experimental Gravity:

|  |
| --- |
| 25 g/mLSynQuest1100-J-03  |
| 2. 629 g/mLAlfa AesarA10954  |
| 2. 6293 g/mLSynQuest1100-J-03  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 492Alfa AesarA10954  |
| 1. 4895SynQuest9195, 1100-J-03  |

* Miscellaneous

## Safety:

|  |
| --- |
| 26-37Alfa AesarA10954  |
| 36/37/38Alfa AesarA10954  |
| H315-H319-H335Alfa AesarA10954  |
| P261-P280-P305+P351+P338-P304+P340-P405-P501aAlfa AesarA10954  |
| R23/24/25, R35/37/38SynQuest1100-J-03  |
| S13, S20, S23, S24/25, S26, S36/37/39, S45SynQuest1100-J-03  |
| Very Toxic/Light SensitiveSynQuest9195  |
| Very Toxic/Light Sensitive/IrritantSynQuest1100-J-03  |
| WarningAlfa AesarA10954  |
| WARNING: Irritates lungs, eyes, skinAlfa AesarA10954  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 790 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 27 mm; Column length: 100 m; Column type: Capillary; Start T: 140 C; CAS no: 354654; Active phase: OV-101; Data type: Kovats RI; Authors: Boneva, S.; Kotov, St., Separation and Identification of . alpha.,. omega.-Diidoperfluoroalkanes in Gas Chromatography, Chromatographia, 25(8), 1988, 735-736.)NIST Spectranist ri  |
| 791 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 27 mm; Column length: 100 m; Column type: Capillary; Start T: 150 C; CAS no: 354654; Active phase: OV-101; Data type: Kovats RI; Authors: Boneva, S.; Kotov, St., Separation and Identification of . alpha.,. omega.-Diidoperfluoroalkanes in Gas Chromatography, Chromatographia, 25(8), 1988, 735-736.)NIST Spectranist ri  |
| 794 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 27 mm; Column length: 100 m; Column type: Capillary; Start T: 160 C; CAS no: 354654; Active phase: OV-101; Data type: Kovats RI; Authors: Boneva, S.; Kotov, St., Separation and Identification of . alpha.,. omega.-Diidoperfluoroalkanes in Gas Chromatography, Chromatographia, 25(8), 1988, 735-736.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 2. 9±0. 1 g/cm 3  |
| Boiling Point:  | 111. 0±8. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 27. 3±0. 2 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 33. 5±3. 0 kJ/mol  |
| Flash Point:  | 36. 0±5. 6 °C  |
| Index of Refraction:  | 1. 537  |
| Molar Refractivity:  | 37. 8±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 1  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 4. 37  |
| ACD/LogD (pH 5. 5):  | 3. 49  |
| ACD/BCF (pH 5. 5):  | 263. 37  |
| ACD/KOC (pH 5. 5):  | 1880. 37  |
| ACD/LogD (pH 7. 4):  | 3. 49  |
| ACD/BCF (pH 7. 4):  | 263. 37  |
| ACD/KOC (pH 7. 4):  | 1880. 37  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 15. 0±0. 5 10 -24 cm 3  |
| Surface Tension:  | 32. 0±3. 0 dyne/cm  |
| Molar Volume:  | 121. 1±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. 79Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 160. 28 (Adapted Stein & Brown method)Melting Pt (deg C): -28. 81 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 26. 3 (Mean VP of Antoine & Grain methods)BP (exp database): 112 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 6165log Kow used: 3. 79 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 8. 0921 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 78E-002 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 986E+001 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 79 (KowWin est)Log Kaw used: 0. 443 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 3. 347Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2112Biowin2 (Non-Linear Model) : 0. 0042Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 1. 9930 (months )Biowin4 (Primary Survey Model) : 3. 0304 (weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 1357Biowin6 (MITI Non-Linear Model): 0. 0000Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 1676Ready 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): 3. 31E+003 Pa (24. 8 mm Hg)Log Koa (Koawin est ): 3. 347Kp (particle/gas partition coef. (m3/ug)): Mackay model : 9. 07E-010 Octanol/air (Koa) model: 5. 46E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 28E-008 Mackay model : 7. 26E-008 Octanol/air (Koa) model: 4. 37E-008 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): 5. 27E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 224. 7Log Koc: 2. 352 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. 219 (BCF = 165. 4)log Kow used: 3. 79 (estimated)Volatilization from Water: Henry LC: 0. 0678 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 936 hoursHalf-Life from Model Lake : 178. 8 hours (7. 452 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 96. 67 percentTotal biodegradation: 0. 06 percentTotal sludge adsorption: 12. 32 percentTotal to Air: 84. 29 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 33. 6 1e+005 1000 Water 32. 9 1. 44e+003 1000 Soil 27. 7 2. 88e+003 1000 Sediment 5. 87 1. 3e+004 0 Persistence Time: 255 hr

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