1,2-diiodoperfluoroethane c2f4i2 structure

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Contents

Molecular Formula	$C_2F_4I_2$
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	37. 8±0. 3 cm ^{3}

Refractivity	
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.

4895SynQuest919

5, 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,

R35/37/38SynQues

t1100-J-03

S13, S20, S23,

S24/25, S26,

S36/37/39,

S45SynQuest1100-

J-03

Very Toxic/Light

SensitiveSynQuest

9195

Very Toxic/Light

Sensitive/IrritantSy

nQuest1100-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.-

Diidoperfluoroalkan

es 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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