Trifluoroethylamine c2h4f3n structure

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Molecular Formula	$C_2H_4F_3N$
Average mass	99. 055 Da
Density	1. 2±0. 1 g/cm ^{3}
Boiling Point	36. 0±35. 0 °C at 760 mmHg
Flash Point	-16. 7±0. 0 °C

Molar Refractivity	15. 3±0. 3 cm ^{3}
Polarizability	6. 1±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	16. 5±3. 0 dyne/cm
Molar Volume	81. 6±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties
  - **Experimental Boiling Point:**

    36-38 °CAlfa Aesar

    37-38 °CManchester OrganicsE19400

    37-38 °CMatrix Scientific

    36-38 °CAlfa AesarB20789

    37-38 °CMatrix Scientific003711

36-37 °CSynQuest26745,

3130-3-04

37-38 °COakwood003057

36-37

°CLabNetworkLN00008843

- **Experimental Optical Rotation:**

1. 301Matrix

Scientific003711

- **Experimental Vapor Pressure:**

450 mmHgSynQuest

450 °CSynQuest26745

450 mmHgSynQuest26745,

3130-3-04

- **Experimental Flash Point:**

-16 °CAlfa Aesar

-16 °CAlfa Aesar

-16 °F (-26. 6667 °C)Alfa

AesarB20789

-16 °CSynQuest26745, 3130-3-

04

-16 °COakwood003057

-17 °CLabNetworkLN00008843

- **Experimental Gravity:**

25 g/mLSynQuest3130-3-04

1. 245 g/mLAlfa AesarB20789

1. 245 g/mLMatrix

Scientific003711

1. 259 g/mLSynQuest3130-3-

04

1. 245 g/mLOakwood003057

1. 245 g/mLFluorochem

1. 245 g/lFluorochem003057

- **Experimental Refraction Index:**

1. 295Alfa AesarB20789

1. 301Matrix

Scientific003711

1. 295SynQuest26745,

3130-3-04

- Miscellaneous

  - **Appearance:**

    Not AvailableNovochemy[NC-30406]

  - **Safety:**

    11/20/1934Alfa AesarB20789

    11/20/1934 12: 00: 00 AMAlfa AesarB20789

    11-20-34Alfa AesarB20789

    20/21/22Novochemy[NC-30406]

    20/21/36/37/39Novochemy[NC-30406]

    3Alfa AesarB20789

    3-9-16-26-36/37/39-45Alfa AesarB20789

    DangerAlfa AesarB20789

    DANGER: FLAMMABLE, CORROSIVE, burns skin and eyesAlfa AesarB20789

    GHS07; GHS09Novochemy[NC-30406]

H225-H314-H332Alfa AesarB20789

H304; H403Novochemy[NC-30406]

Highly Flammable/Corrosive/Harmful/Keep ColdSynQuest26745, 3130-3-04

IRRITANT-HARMFUL, FLAMMABLE, CORROSIVEMatrix Scientific003711

P210-P260-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarB20789

P305+P351+P338; P376; P270Novochemy[NC-30406]

R11, 20/21/22, R36/37/38SynQuest26745, 3130-3-04

R11, R22, R34, R52/53SynQuest3130-3-04

R22Novochemy[NC-30406]

S3/7, S15, S16, S24/25, S36/37/39, S45SynQuest26745, 3130-3-04

S3/7, S16, S24/25, S26, S36/37/39, S45, S61SynQuest3130-3-04

WarningNovochemy[NC-30406]

- Gas Chromatography

• Retention Index (Kovats):

297 (estimated with error: 89)NIST Spectramainlib_118517,

replib_238208

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

Density:	1. 2±0. 1 g/cm ^{3}
Boiling Point:	36. 0±35. 0 °C at 760 mmHg
Vapour Pressure:	501. 5±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	28. 1±3. 0 kJ/mol
Flash Point:	-16. 7±0. 0 °C
Index of Refraction:	1. 301
Molar Refractivity:	15. 3±0. 3 cm ^{3}
#H bond acceptors:	1
#H bond donors:	2
#Freely Rotating Bonds:	1
#Rule of 5 Violations:	0
ACD/LogP:	0. 24
ACD/LogD (pH 5. 5):	-0. 12
ACD/BCF (pH 5. 5):	1. 00

ACD/KOC (pH 5. 5):	15. 15
ACD/LogD (pH 7. 4):	0. 16
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	28. 92
Polar Surface Area:	26 Å ^{2}
Polarizability:	6. 1±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	16. 5±3. 0 dyne/cm
Molar Volume:	81. 6±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) = 0. 27Log Kow (Exper. database match) = 0. 24Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 18. 12 (Adapted Stein & Brown method)Melting Pt (deg C): -88. 25 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 475 (Mean VP of Antoine & Grain methods)BP (exp database): 37. 5 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 7. 478e+005log Kow used: 0. 24 (expkow database)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1. 4062e+005 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 92E-005 atm-m3/moleGroup Method: 2. 08E-005 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 8. 279E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 24 (exp database)Log Kaw used: -2. 490 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 730Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 3338Biowin2 (Non-Linear Model) : 0. 0494Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 4917 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4737 (days-weeks)MITI

Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5523Biowin6 (MITI Non-Linear Model): 0. 0000Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 0394Ready 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. 32E+004 Pa (474 mm Hg)Log Koa (Koawin est): 2. 730Kp (particle/gas partition coef. (m3/ug)): Mackay model : 4. 75E-011 Octanol/air (Koa) model: 1. 32E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 71E-009 Mackay model : 3. 8E-009 Octanol/air (Koa) model: 1. 05E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 6167 E-12 cm3/molecule-secHalf-Life = 17. 343 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 76E-009 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 72. 59Log Koc: 1. 861 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. 500 (BCF = 3. 162)log Kow used: 0. 24 (expkow database)Volatilization from Water: Henry LC: 2. 08E-005 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 29. 03 hours (1. 21 days)Half-Life from Model Lake : 400. 2 hours (16. 67 days)Removal In Wastewater Treatment: Total removal: 2. 98 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 74 percentTotal to Air: 1. 14 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 7. 07 276 1000 Water 51. 4 900 1000 Soil 41. 4 1. 8e+003 1000 Sediment 0. 1 8. 1e+003 0 Persistence Time: 512 hr

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