Acetaldehyde ammonia trimer c6h15n3 structure

ASSIGN BUSTER

Contents

Molecular Formula	$C_6H_{15}N_3$
Average mass	129. 203 Da
Density	0. 8±0. 1 g/cm ^{3}
Boiling Point	110. 0±0. 0 °C at 760 mmHg
Flash Point	15. 4±13. 5 °C
Molar Refractivity	38. 0±0. 3 cm ^{3}
Polarizability	15. 1±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	22. 5±3. 0 dyne/cm
Molar	154. 5±3.

Volume 0 cm^3

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

Experimental Melting Point:

93-96 °CAlfa Aesar

93-96 °CAlfa

AesarL12265

Experimental Boiling Point:

110 °C

(Decompos

es)Alfa

Aesar

110 °C

(Decompos

es)Alfa

AesarL1226

5

- **Experimental Gravity:**

  0. 852

  g/mLAlfa

  AesarL1226

  5

- Miscellaneous

- **Safety:**

  26-37Alfa

  AesarL1226

  5

  36/37/38Alf

  a

  AesarL1226

  5

  DANGER:

  FLAMMABLE

  , irritates

  skin, eyes,

  lungsAlfa

  AesarL1226

  5

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

Density:	0. 8±0. 1 g/cm ^{3}
Boiling Point:	110. 0±0. 0 °C at 760 mmHg
Vapour Pressure:	24. 2±0. 2 mmHg at 25°C
Enthalpy of Vaporization:	34. 9±3. 0 kJ/mol
Flash Point:	15. 4±13. 5 °C
Index of Refraction:	1. 407
Molar Refractivity:	38. 0±0. 3 cm ^{3}
#H bond acceptors:	3
#H bond donors:	3
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	0. 43
ACD/LogD (pH 5. 5):	-2. 82
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00
ACD/LogD (pH 7. 4):	-1. 56

ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	1. 00
Polar Surface Area:	36 Å ^{2}
Polarizability:	15. 1±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	22. 5±3. 0 dyne/cm
Molar Volume:	154. 5±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) = -1. 53Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 237. 87 (Adapted Stein & Brown method)Melting Pt (deg C): 68. 48 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0193 (Modified Grain method)Subcooled liquid VP: 0. 0495 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1e+006log Kow used: -1. 53 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 09E-005 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 281E-009 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -1. 53 (KowWin est)Log Kaw used: -3. 068 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 1. 538Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 1475Biowin2 (Non-Linear Model) : 0. 9891Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9870 (weeks)Biowin4 (Primary Survey Model) : 3. 7912 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4662Biowin6 (MITI Non-Linear Model): 0. 0841Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 2476Ready 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. 6 Pa (0. 0495 mm Hg)Log Koa (Koawin est): 1. 538Kp (particle/gas partition coef. (m3/ug)): Mackay model : 4. 55E-007 Octanol/air (Koa) model: 8. 47E-012 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 64E-005 Mackay model : 3. 64E-005 Octanol/air

(Koa) model: 6. 78E-010 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 692. 8737 E-12 cm3/molecule-secHalf-Life = 0. 015 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 11. 115 MinOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 64E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 126. 4Log Koc: 2. 102 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: -1. 53 (estimated)Volatilization from Water: Henry LC: 2. 09E-005 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 33 hours (1. 375 days)Half-Life from Model Lake : 455. 3 hours (18. 97 days)Removal In Wastewater Treatment: Total removal: 2. 97 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 74 percentTotal to Air: 1. 15 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0771 0. 371 1000 Water 49. 5 360 1000 Soil 50. 3 720 1000 Sediment 0. 0906 3. 24e+003 0 Persistence Time: 296 hr

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