6-apb c11h13no structure

Contents

Molecular Formula	$C_{11}H_{13}NO$
Average mass	175. 227 Da
Density	1. 1±0. 1 g/cm ^{3}
Boiling Point	277. 1±15. 0 °C at 760 mmHg
Flash Point	121. 4±20. 4 °C
Molar Refractivity	54. 1±0. 3 cm ^{3}
Polarizability	21. 4±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	42. 5±3. 0 dyne/cm
Molar Volume	159. 7±3. 0 cm ^{3}

- **Appearance:**

  Not AvailableNovochemy[NC-35574]

- **Safety:**

  20/21/22Novochemy[NC-35574]

  20/21/36/37/39Novochemy[NC-35574]

  GHS07; GHS09Novochemy[NC-35574]

  H332; H403Novochemy[NC-35574]

  P309+P311; P211; P242Novochemy[NC-35574]

  R52/53Novochemy[NC-35574]

  WarningNovochemy[NC-35574]

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

Density:	1. 1±0. 1 g/cm ^{3}
Boiling Point:	277. 1±15. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 6 mmHg at 25°C
Enthalpy of Vaporization:	51. 6±3. 0 kJ/mol

Flash Point:	121. 4±20. 4 °C
Index of Refraction:	1. 592
Molar Refractivity:	54. 1±0. 3 cm^3
#H bond acceptors:	2
#H bond donors:	2
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0
ACD/LogP:	2. 26
ACD/LogD (pH 5. 5):	-0. 76
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00
ACD/LogD (pH 7. 4):	-0. 02
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	2. 02
Polar Surface Area:	39 $Å^2$

Polarizability: $21.4 \pm 0.5 \times 10^{-24}$ cm ^{3}

Surface Tension: 42. 5±3. 0 dyne/cm

Molar Volume: 159. 7±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. 30Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 287. 68 (Adapted Stein & Brown method)Melting Pt (deg C): 72. 81 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00132 (Modified Grain method)Subcooled liquid VP: 0. 00374 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): 6409log Kow used: 2. 30 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1377. 9 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 05E-007 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 4. 749E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 30 (KowWin est)Log Kaw used: -5. 367 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 667Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8726Biowin2 (Non-Linear Model) : 0. 9009Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7615 (weeks)Biowin4 (Primary Survey Model) : 3. 5697 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 1592Biowin6 (MITI Non-Linear Model): 0. 0815Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 1690Ready 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): 0. 499 Pa (0. 00374 mm Hg)Log Koa (Koawin est): 7. 667Kp (particle/gas partition coef. (m3/ug)): Mackay model : 6. 02E-006 Octanol/air (Koa) model: 1. 14E-005 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000217 Mackay model : 0. 000481 Octanol/air (Koa) model: 0. 000911 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 137. 1926 E-12 cm3/molecule-secHalf-Life = 0. 078 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 936 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000349 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 6678Log Koc: 3. 825 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 = 1. 072 (BCF = 11. 8)log Kow used: 2. 30 (estimated)Volatilization from Water: Henry LC: 1. 05E-007 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 7383 hours (307. 6 days)Half-Life from Model Lake : 8. 065E+004 hours (3360 days)Removal In Wastewater Treatment: Total removal: 2. 64 percentTotal biodegradation: 0. 10

percentTotal sludge adsorption: 2. 54 percentTotal to Air: 0. 01 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 185 1. 87 1000 Water 28. 1 360 1000 Soil 71. 6 720 1000 Sediment 0. 145 3. 24e+003 0 Persistence Time: 452 hr

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