2-(2-nitrophenyl)ethanol c8h9no3 structure

ASSIGN BUSTER

Contents

- Retention Index (Kovats):

Molecular Formula	$C_8H_9NO_3$
Average mass	167. 162 Da
Density	1. 3±0. 1 g/cm ^{3}
Boiling Point	267. 0±0. 0 °C at 760 mmHg
Flash Point	129. 6±8. 8 °C
Molar Refractivity	43. 9±0. 3 cm ^{3}
Polarizability	17. 4±0. 5 10^{-24} cm ^{3}
Surface Tension	53. 6±3. 0 dyne/cm
Molar Volume	131. 6±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

Experimental Melting Point:

2 °COxford University

Chemical Safety Data

(No longer

updated)More details

2 °CJean-Claude

Bradley Open Melting

Point Dataset15096,

17599

2 °CSynQuest4754-1-

48

2

°CLabNetworkLN00124

394

Experimental Boiling Point:

267 °COxford

University Chemical

Safety Data (No longer

updated)More details

267 °CMatrix Scientific

267 °CMatrix

Scientific016545

267 °CSynQuest4754-

1-48

267

°CLabNetworkLN00124

394

- **Experimental Flash Point:**

  113 °CSynQuest4754-1-48

  230

  °CLabNetworkLN00124394

- **Experimental Gravity:**

  1. 19 g/mLSynQuest4754-

  1-48

- **Experimental Refraction Index:**

  1. 5637SynQuest4754-

  1-48

- Miscellaneous

- **Appearance:**

  brown liquidOxford University Chemical Safety Data (No longer updated)More details

  Not AvailableNovochemy[NC-21271]

- **Stability:**

  Stable. Incompatible with strong oxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details

- **Safety:**

  20/21/22Novochemy[NC-21271]

  20/21/36/37/39Novochemy[NC-21271]

  GHS07;

GHS09Novochemy[NC-21271]

H304; H332; H403Novochemy[NC-21271]

IRRITANTMatrix Scientific016545

IrritantSynQuest4754-1-48

P332+P313; P305+P351+P338Novochemy[NC-21271]

R22Novochemy[NC-21271]

Treat as potentially harmful. Oxford University Chemical Safety Data (No longer updated)More details

WarningNovochemy[NC-21271]

- Gas Chromatography

  - **Retention Index (Kovats):**

    1531 (estimated with

    error: 89)NIST

    Spectramainlib_291470

    , replib_76339,

    replib_235481

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

Density:	1. 3±0. 1 g/cm ^{3}
Boiling Point:	267. 0±0. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 5 mmHg at 25°C
Enthalpy of Vaporization:	53. 3±3. 0 kJ/mol
Flash Point:	129. 6±8. 8 °C
Index of Refraction:	1. 581
Molar Refractivity:	43. 9±0. 3 cm ^{3}
#H bond acceptors:	4
#H bond donors:	1
#Freely Rotating Bonds:	3

#Rule of 5 Violations:	0
ACD/LogP:	1. 09
ACD/LogD (pH 5. 5):	1. 35
ACD/BCF (pH 5. 5):	6. 29
ACD/KOC (pH 5. 5):	129. 84
ACD/LogD (pH 7. 4):	1. 35
ACD/BCF (pH 7. 4):	6. 29
ACD/KOC (pH 7. 4):	129. 84
Polar Surface Area:	66 Å ^{2}
Polarizability:	17. 4±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	53. 6±3. 0 dyne/cm
Molar Volume:	131. 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) = 1. 38Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 304. 41 (Adapted Stein & Brown method)Melting Pt (deg C): 85. 60 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00107 (Mean VP of Antoine & Grain methods)MP (exp database): 2 deg CBP (exp database): 267 deg CWater

Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1698log Kow used: 1. 38 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 5835 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 14E-009 atm-m3/moleGroup Method: 8. 48E-010 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 386E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 38 (KowWin est)Log Kaw used: -7. 332 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 8. 712Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5763Biowin2 (Non-Linear Model) : 0. 4554Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7453 (weeks-months)Biowin4 (Primary Survey Model) : 3. 5591 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2150Biowin6 (MITI Non-Linear Model): 0. 0515Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2773Ready 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. 147 Pa (0. 0011 mm Hg)Log Koa (Koawin est): 8. 712Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 05E-005 Octanol/air (Koa) model: 0. 000126 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000738 Mackay model : 0. 00163 Octanol/air (Koa) model: 0. 01 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 5. 9152 E-12 cm3/molecule-secHalf-Life = 1. 808 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 21. 699 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 00119 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 34. 01Log Koc: 1. 532 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. 284 (BCF = 0. 5199)log Kow used: 1. 38 (estimated)Volatilization from Water: Henry LC: 8. 48E-010 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 8. 927E+005 hours (3. 72E+004 days)Half-Life from Model Lake : 9. 738E+006 hours (4. 058E+005 days)Removal In Wastewater Treatment: Total removal: 1. 94 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 85 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 01 43. 4 1000 Water 35. 2 900 1000 Soil 64. 7 1. 8e+003 1000 Sediment 0. 0837 8. 1e+003 0 Persistence Time: 1. 14e+003 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop