

# [2-(2-nitrophenyl)ethanol c8h9no3 structure](https://assignbuster.com/2-2-nitrophenylethanol-c8h9no3-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 8 H 9 NO 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| 2 °COxford University Chemical Safety Data (No longer updated)More details  |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 °CLabNetworkLN00124394  |

## 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| 267 °COxford University Chemical Safety Data (No longer updated)More details  |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 °CLabNetworkLN00124394  |

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| brown liquidOxford University Chemical Safety Data (No longer updated)More details  |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 Oxford University Chemical Safety Data (No longer updated)More details  |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 Oxford University Chemical Safety Data (No longer updated)More details  |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

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* 1-Click Scaffold Hop