

# [6-apb c11h13no structure](https://assignbuster.com/6-apb-c11h13no-structure/)

Contents

* Safety:

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| 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  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Miscellaneous

## Appearance:

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| Not AvailableNovochemy[NC-35574]  |

## Safety:

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| 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

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| 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  |

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| 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±0. 5 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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