

# [Dicyclohexylamine c12h23n structure](https://assignbuster.com/dicyclohexylamine-c12h23n-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 12 H 23 N  |
| Average mass  | 181. 318 Da  |
| Density  | 0. 9±0. 1 g/cm 3  |
| Boiling Point  | 256. 1±8. 0 °C at 760 mmHg  |
| Flash Point  | 96. 1±0. 0 °C  |
| Molar Refractivity  | 57. 1±0. 4 cm 3  |
| Polarizability  | 22. 6±0. 5 10 -24 cm 3  |
| Surface Tension  | 33. 2±5. 0 dyne/cm  |
| Molar Volume  | 198. 3±5. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -2 °CAlfa Aesar  |
| -1 °COxford University Chemical Safety Data (No longer updated)More details  |
| -1 °CJean-Claude Bradley Open Melting Point Dataset15987  |
| -0. 1 °CJean-Claude Bradley Open Melting Point Dataset20653  |
| -2 °CJean-Claude Bradley Open Melting Point Dataset14297, 6814  |
| -2 °CAlfa AesarA15671  |
| -2 °COakwood098446  |

## Experimental Boiling Point:

|  |
| --- |
| 256 °CAlfa Aesar  |
| 256 °COxford University Chemical Safety Data (No longer updated)More details  |
| 256 °CAlfa AesarA15671  |
| 255-257 °COakwood098446  |

## Experimental Flash Point:

|  |
| --- |
| 99 °CAlfa Aesar  |
| 99 °COxford University Chemical Safety Data (No longer updated)More details  |
| 99 °CAlfa Aesar  |
| 99 °F (37. 2222 °C)Alfa AesarA15671  |
| 96 °COakwood098446  |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLMerck Millipore1441  |
| 20 g/lMerck Millipore1441, 802948  |
| 0. 913 g/mLAlfa AesarA15671  |
| 0. 912 g/mLOakwood098446  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 4842Alfa AesarA15671  |

* Miscellaneous

## Appearance:

|  |
| --- |
| colourless or light yellow liquidOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

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 Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 373 mg kg-1, SCU-MUS LD50 135 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 1/2-26-36/37/39-45-60-61Alfa AesarA15671  |
| 22-34-50/53Alfa AesarA15671  |
| 26-36/37/39-45-60-61Alfa AesarA15671  |
| 8Alfa AesarA15671  |
| DangerAlfa AesarA15671  |
| DANGER: CORROSIVE, burns skin and eyesAlfa AesarA15671  |
| H314-H400-H410-H302Alfa AesarA15671  |
| P260-P303+P361+P353-P305+P351+P338-P301+P330+P331-P405-P501aAlfa AesarA15671  |
| Safety glasses, adequate ventilation. Oxford University Chemical Safety Data (No longer updated)More details  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1540 (estimated with error: 83)NIST Spectramainlib\_290817, replib\_7528, replib\_228971  |
| 1431. 48 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: Capillary; Start T: 170 C; CAS no: 101837; Active phase: DB-1; Carrier gas: He; Phase thickness: 3 um; Data type: Kovats RI; Authors: Kuhn, E. R., Selectivity vs. polarity: the fundamentals of chromatographic separation, J. Sep. Sci., 24, 2001, 473-476.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1392 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 80 C; End T: 260 C; CAS no: 101837; Active phase: Ultra-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Okumura, T., retention indices of environmental chemicals on methyl silicone capillary column, Journal of Environmental Chemistry (Japan), 1(2), 1991, 333-358.)NIST Spectranist ri  |
| 1437 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri  |
| 1442 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri  |
| 1444 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri  |
| 1663 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Carbowax 20M / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri  |
| 1673 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Carbowax 20M / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri  |
| 1683 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Carbowax 20M / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 1408 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 12 m; Column type: Capillary; Description: 120C=> 8C/min=> 270C=> 25C/min=> 300C; CAS no: 101837; Active phase: BP-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Stowell, A.; Wilson, L. W., A simple approach to the interlaboratory transfer of drug retention indices determined by temperature programmed capillary gas chromatography, J. Forensic Sci., 32(5), 1987, 1214-1220.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 0. 9±0. 1 g/cm 3  |
| Boiling Point:  | 256. 1±8. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 5 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 49. 4±3. 0 kJ/mol  |
| Flash Point:  | 96. 1±0. 0 °C  |
| Index of Refraction:  | 1. 488  |
| Molar Refractivity:  | 57. 1±0. 4 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 1  |
| #Freely Rotating Bonds:  | 2  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 3. 69  |
| ACD/LogD (pH 5. 5):  | 0. 58  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 1. 89  |
| ACD/LogD (pH 7. 4):  | 0. 62  |
| ACD/BCF (pH 7. 4):  | 1. 00  |
| ACD/KOC (pH 7. 4):  | 2. 11  |
| Polar Surface Area:  | 12 Å 2  |
| Polarizability:  | 22. 6±0. 5 10 -24 cm 3  |
| Surface Tension:  | 33. 2±5. 0 dyne/cm  |
| Molar Volume:  | 198. 3±5. 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) = 4. 37Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 256. 50 (Adapted Stein & Brown method)Melting Pt (deg C): 27. 68 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 02 (Mean VP of Antoine & Grain methods)MP (exp database): -0. 1 deg CBP (exp database): 255. 8 deg CVP (exp database): 3. 38E-02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 103. 1log Kow used: 4. 37 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1896. 6 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 50E-005 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 4. 628E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 37 (KowWin est)Log Kaw used: -2. 648 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 018Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8151Biowin2 (Non-Linear Model) : 0. 8240Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8229 (weeks )Biowin4 (Primary Survey Model) : 3. 6294 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4281Biowin6 (MITI Non-Linear Model): 0. 2917Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 1079Ready 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): 4. 51 Pa (0. 0338 mm Hg)Log Koa (Koawin est ): 7. 018Kp (particle/gas partition coef. (m3/ug)): Mackay model : 6. 66E-007 Octanol/air (Koa) model: 2. 56E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 4E-005 Mackay model : 5. 33E-005 Octanol/air (Koa) model: 0. 000205 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 131. 7220 E-12 cm3/molecule-secHalf-Life = 0. 081 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 974 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 3. 86E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 256. 3Log Koc: 2. 409 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 = 2. 662 (BCF = 459. 5)log Kow used: 4. 37 (estimated)Volatilization from Water: Henry LC: 5. 5E-005 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 15. 71 hoursHalf-Life from Model Lake : 284. 3 hours (11. 84 days)Removal In Wastewater Treatment: Total removal: 50. 04 percentTotal biodegradation: 0. 46 percentTotal sludge adsorption: 48. 18 percentTotal to Air: 1. 40 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 219 1. 95 1000 Water 20. 6 360 1000 Soil 73. 3 720 1000 Sediment 5. 9 3. 24e+003 0 Persistence Time: 471 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop