

# [Dipropylamine c6h15n structure](https://assignbuster.com/dipropylamine-c6h15n-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 6 H 15 N  |
| Average mass  | 101. 190 Da  |
| Density  | 0. 7±0. 1 g/cm 3  |
| Boiling Point  | 108. 8±0. 0 °C at 760 mmHg  |
| Flash Point  | 3. 9±0. 0 °C  |
| Molar Refractivity  | 33. 4±0. 3 cm 3  |
| Polarizability  | 13. 3±0. 5 10 -24 cm 3  |
| Surface Tension  | 23. 0±3. 0 dyne/cm  |
| Molar Volume  | 136. 4±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -63 °CTCID0930  |
| -40 °COxford University Chemical Safety Data (No longer updated)More details  |
| -40 °CJean-Claude Bradley Open Melting Point Dataset16029  |
| -63 °CJean-Claude Bradley Open Melting Point Dataset13348, 20116, 6950  |
| -63 °CAlfa AesarL15808  |
| -63 °CSynQuest3131-1-18  |
| -63 °CLabNetworkLN00225878  |
| -63 °CFooDBFDB003929  |

## Experimental Boiling Point:

|  |
| --- |
| 108-110 °COxford University Chemical Safety Data (No longer updated)More details  |
| 109-110 °CAlfa AesarL15808  |
| 105-110 °CSynQuest3131-1-18  |
| 105-110 °C (Literature)LabNetworkLN00225878  |

## Experimental Flash Point:

|  |
| --- |
| 7 °COxford University Chemical Safety Data (No longer updated)More details  |
| 7 °CAlfa Aesar  |
| 7 °F (-13. 8889 °C)Alfa AesarL15808  |
| 7 °CSynQuest3131-1-18  |
| 7 °CLabNetworkLN00225878  |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLMerck Millipore1109  |
| 20 g/lMerck Millipore1109, 803548  |
| 0. 738 g/mLAlfa AesarL15808  |
| 0. 74 g/mLSynQuest3131-1-18  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 405Alfa AesarL15808  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| -63 °CTCI  |
| -63 °CTCID0930  |

* Miscellaneous

## Appearance:

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| colourless liquidOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

|  |
| --- |
| Stable. Highly flammable. Incompatible with strongoxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 300 mg kg-1, SKN-RBT LD50 925 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 1/2-16-26-36/37/39-45Alfa AesarL15808  |
| 11-20/21/22-35Alfa AesarL15808  |
| 16-26-36/37/39-45Alfa AesarL15808  |
| 3Alfa AesarL15808  |
| CORROSIVE / FLAMMABLE / HARMFULAlfa AesarL15808  |
| DangerAlfa AesarL15808  |
| H225-H314-H302-H312-H332Alfa AesarL15808  |
| Highly Flammable/Corrosive/Harmful/Lachrymatory/HygroscopicSynQuest3131-1-18  |
| P210-P260-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarL15808  |
| Safety glasses, gloves (rubber), good ventilation. Removesources of ignition from the working area. Oxford University Chemical Safety Data (No longer updated)More details  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 816 (estimated with error: 83)NIST Spectramainlib\_233533, replib\_228163, replib\_290912  |
| 750 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 142847; Active phase: PMS-100; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri  |
| 752 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 130 C; CAS no: 142847; Active phase: PMS-100; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 142847; Active phase: PMS-100; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri  |
| 742. 6 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 3. 3 m; Column type: Packed; Start T: 130 C; CAS no: 142847; Active phase: C78, Branched paraffin; Carrier gas: He; Data type: Kovats RI; Authors: Dallos, A.; Sisak, A.; Kulcsar, Z.; Kovats, E., Pair-wise interactions by gas chromatography VII. Interaction free enthalpies of solutes with secondary alcohol groups, J. Chromatogr. A, 904, 2000, 211-242., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 3. 3 m; Column type: Packed; Start T: 130 C; CAS no: 142847; Active phase: C78, Branched paraffin; Substrate: Chromosorb G HP; Data type: Kovats RI; Authors: Reddy, K. S.; Dutoit, J.-Cl.; Kovats, E. sz., Pair-wise interactions by gas chromatography. I. Interaction free enthalpies of solutes with non-associated primary alcohol groups, J. Chromatogr., 609, 1992, 229-259.)NIST Spectranist ri  |
| 744 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 3. 7 m; Column type: Packed; Start T: 130 C; CAS no: 142847; Active phase: Apolane; Data type: Kovats RI; Authors: Dutoit, J., Gas chromatographic retention behaviour of some solutes on structurally similar polar and non-polar stationary phases, J. Chromatogr., 555, 1991, 191-204.)NIST Spectranist ri  |
| 746 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 26 m; Column type: Packed; Start T: 130 C; CAS no: 142847; Active phase: Apiezon L; Substrate: Teflon-Haloport; Data type: Kovats RI; Authors: Landault, C.; Guiochon, G., Separation des amines par chromatographie gaz-liquide en utilisant le teflon comme support, J. Chromatogr., 13, 1964, 327-336., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 7 m; Column type: Packed; Start T: 100 C; CAS no: 142847; Active phase: Apiezon L; Carrier gas: N2; Substrate: Chromosorb GAW; Data type: Kovats RI; Authors: Golovnya, R. V.; Zhuravleva, N. L.; Svetlova, N. I.; Grigor’eva, D. N., Gas-chromatographic separation of secondary normal alphatic amines, J. Anal. Chem. USSR (Engl. Transl.), 35(10), 1980, 1280-1285, In original 1976-1981., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 7 m; Column type: Packed; Start T: 100 C; CAS no: 142847; Active phase: Apiezon L; Substrate: Chromosorb G AW (80-100 mesh); Data type: Kovats RI; Authors: Golovnya, R. V.; Zhuravleva, I. L.; Svetlova, I.; Terenina, M. B.; Gutnik, S. B., Calculation of gas chromatographic retention indices of secondary amines from structural increments, Zh. Anal. Khim., 37, 1982, 294-300.)NIST Spectranist ri  |
| 748 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 100 C; CAS no: 142847; Active phase: Apiezon L; Data type: Kovats RI; Authors: Golovnya, R. V.; Zhuravleva, I. L., Gas Chromatographic Method of Identification of n-Aliphatic Amines Through the Use of Donor-Acceptor Interaction with Phosphate, Chromatographia, 6(12), 1973, 508-513.)NIST Spectranist ri  |
| 894 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 200 C; CAS no: 142847; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri  |
| 900 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 179 C; CAS no: 142847; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri  |
| 901 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 120 C; CAS no: 142847; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri  |
| 904 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 142847; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri  |
| 905 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 152 C; CAS no: 142847; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri  |
| 910 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 142847; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 748 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 142847; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Chen, Y.; Feng, C., QSPR study on gas chromatography retention index of some organic pollutants, Comput. Appl. Chem. (China), 24(10), 2007, 1404-1408.)NIST Spectranist ri  |
| 745 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 142847; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Zenkevich, I. G., Dependence of Gas Chromatographic Retention Indices on Dynamics Molecular Characteristics, Zh. Fiz. Khim., 73(5), 1999, 905-910, In original 905-910.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 0. 7±0. 1 g/cm 3  |
| Boiling Point:  | 108. 8±0. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 25. 5±0. 2 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 33. 5±0. 0 kJ/mol  |
| Flash Point:  | 3. 9±0. 0 °C  |
| Index of Refraction:  | 1. 405  |
| Molar Refractivity:  | 33. 4±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 1  |
| #Freely Rotating Bonds:  | 4  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 1. 70  |
| ACD/LogD (pH 5. 5):  | -1. 38  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 1. 00  |
| ACD/LogD (pH 7. 4):  | -1. 25  |
| ACD/BCF (pH 7. 4):  | 1. 00  |
| ACD/KOC (pH 7. 4):  | 1. 00  |
| Polar Surface Area:  | 12 Å 2  |
| Polarizability:  | 13. 3±0. 5 10 -24 cm 3  |
| Surface Tension:  | 23. 0±3. 0 dyne/cm  |
| Molar Volume:  | 136. 4±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. 79Log Kow (Exper. database match) = 1. 67Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 116. 83 (Adapted Stein & Brown method)Melting Pt (deg C): -54. 28 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 25 (Mean VP of Antoine & Grain methods)MP (exp database): -63 deg CBP (exp database): 109. 3 deg CVP (exp database): 2. 01E+01 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 4. 429e+004log Kow used: 1. 67 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 3. 51e+004 mg/L (25 deg C)Exper. Ref: KUHNE, R ET AL. (1995)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 39761 mg/LWat Sol (Exper. database match) = 35100. 00Exper. Ref: KUHNE, R ET AL. (1995)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 17E-005 atm-m3/moleGroup Method: 5. 23E-005 atm-m3/moleExper Database: 5. 10E-05 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 7. 516E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 67 (exp database)Log Kaw used: -2. 681 (exp database)Log Koa (KOAWIN v1. 10 estimate): 4. 351Log Koa (experimental database): 3. 590Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8532Biowin2 (Non-Linear Model) : 0. 9359Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0000 (weeks )Biowin4 (Primary Survey Model) : 3. 7450 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6429Biowin6 (MITI Non-Linear Model): 0. 7459Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 9582Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 2. 68E+003 Pa (20. 1 mm Hg)Log Koa (Exp database): 3. 590Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 12E-009 Octanol/air (Koa) model: 9. 55E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 4. 04E-008 Mackay model : 8. 96E-008 Octanol/air (Koa) model: 7. 64E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 87. 0003 E-12 cm3/molecule-secHalf-Life = 0. 123 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 475 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 6. 5E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 155. 1Log Koc: 2. 191 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. 586 (BCF = 3. 854)log Kow used: 1. 67 (expkow database)Volatilization from Water: Henry LC: 5. 1E-005 atm-m3/mole (Henry experimental database)Half-Life from Model River: 12. 57 hoursHalf-Life from Model Lake : 221. 5 hours (9. 23 days)Removal In Wastewater Treatment: Total removal: 4. 65 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 90 percentTotal to Air: 2. 66 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 567 2. 95 1000 Water 36. 6 360 1000 Soil 62. 7 720 1000 Sediment 0. 0965 3. 24e+003 0 Persistence Time: 326 hr

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* 1-Click Scaffold Hop