

# [Dimethylamine c2h7n structure](https://assignbuster.com/dimethylamine-c2h7n-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 2 H 7 N  |
| Average mass  | 45. 084 Da  |
| Density  | 0. 6±0. 1 g/cm 3  |
| Boiling Point  | 6. 1±3. 0 °C at 760 mmHg  |
| Flash Point  | -56. 1±8. 8 °C  |
| Molar Refractivity  | 14. 9±0. 3 cm 3  |
| Polarizability  | 5. 9±0. 5 10 -24 cm 3  |
| Surface Tension  | 15. 5±3. 0 dyne/cm  |
| Molar Volume  | 70. 4±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -92 °COxford University Chemical Safety Data (No longer updated)More details  |
| -92 °CJean-Claude Bradley Open Melting Point Dataset13102, 16011  |
| -92. 2 °CJean-Claude Bradley Open Melting Point Dataset22407  |
| -37 °CSynQuest66318, 3131-1-X3  |
| -93 °CLabNetworkLN00164054  |
| -96 °CFooDBFDB012589  |

## Experimental Boiling Point:

|  |
| --- |
| 44 F (6. 6667 °C)NIOSHIP8750000  |
| 7. 4 °COxford University Chemical Safety Data (No longer updated)More details  |
| 60 °CAlfa AesarH27665  |
| 52 °CSynQuest66318, 3131-1-X3  |
| 60 °COakwood[051280]  |
| 60 °CLabNetworkLN00164054  |
| 7 °CFooDBFDB012589  |

## Experimental Ionization Potent:

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| --- |
| 8. 24 EvNIOSHIP8750000  |

## Experimental Vapor Pressure:

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| --- |
| 1. 7 atm (1292 mmHg)NIOSHIP8750000  |

## Experimental LogP:

|  |
| --- |
| -0. 38Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s  |

## Experimental Flash Point:

|  |
| --- |
| 20 F (-6. 6667 °C)(Gas, Liquid, None)NIOSHIP8750000  |
| -6 °COxford University Chemical Safety Data (No longer updated)More details  |
| 5 °CAlfa Aesar  |
| -36 °CAlfa Aesar  |
| 15 °CAlfa Aesar  |
| 5 °F (-15 °C)Alfa AesarH27261  |
| 15 °F (-9. 4444 °C)Alfa Aesar43261, 31458  |
| -36 °F (-37. 7778 °C)Alfa AesarH27665  |
| 16 °CSynQuest66318, 3131-1-X3  |
| 16 °COakwood[044754]  |
| -36 °COakwood[051280]  |
| -36 °CLabNetworkLN00164054  |

## Experimental Freezing Point:

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| -134 F (-92. 2222 °C)NIOSHIP8750000  |

## Experimental Gravity:

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| 0. 775 g/mLAlfa AesarH27261  |
| 0. 89 g/mLAlfa Aesar43261, 31458  |
| 0. 85 g/mLAlfa AesarH27665  |
| 0. 89 g/mLSynQuest3131-1-X3  |
| 0. 89 g/mLOakwood[044754]  |
| 0. 85 g/mLOakwood[051280]  |
| 0. 89 g/mLFluorochem044754  |
| 0. 85 g/mLFluorochem  |
| 0. 775 g/lFluorochem044754  |
| 0. 85 g/lFluorochem051280  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 37Alfa Aesar43261, 31458  |
| 1. 37SynQuest66318, 3131-1-X3  |

* Miscellaneous

## Appearance:

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| Colorless gas with an ammonia- or fish-like odor. [Note: A liquid below 44F. Shipped as a liquefied compressed gas.]NIOSHIP8750000  |
| colourless gas with strong ammonia-like smellOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

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| Stable. Generally used as a solution in water at concentrationsup to around 40%. Extremely flammable in the pure form. Incompatible with strongoxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

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| ORL-RAT LD50 698 mg kg-1, ORL-GPG LD50 240 mg kg-1, IPR-MUS LD50 736 mg kg-1, ORL-RBT LD50 240 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 11-19-36/37Alfa AesarH27665  |
| 11-20-37/38-41Alfa Aesar31458, 43261  |
| 11-23/24/25-37/38-39/23/24/25-41Alfa AesarH27261  |
| 3Alfa Aesar31458, 43261, H27261, H27665  |
| 4-9-16-20-23-26-27-33-36/37/39-45-60Alfa AesarH27261  |
| 9-16-23-26-33-39-60Alfa AesarH27665  |
| 9-16-23-26-36/37/39Alfa Aesar31458, 43261  |
| DangerAlfa Aesar31458, 43261, H27261, H27665  |
| DANGER: FLAMMABLE, CORROSIVE, burns skin and eyesAlfa Aesar31458, 43261  |
| H225-H311-H331-H370-H314Alfa AesarH27261  |
| H225-H314-H351-H335-H336-EUH019Alfa AesarH27665  |
| H225-H331-H318-H302-H315-H335Alfa Aesar31458, 43261  |
| Highly Flammable/Corrosive/HygroscopicSynQuest3131-1-X3, 66318  |
| P210-P260-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarH27665  |
| P210-P261-P303+P361+P353-P305+P351+P338-P405-P501aAlfa Aesar31458, 43261  |
| P210-P303+P361+P353-P305+P351+P338-P361-P405-P501aAlfa AesarH27261  |
| Safety glasses, gloves, good ventilation. Oxford University Chemical Safety Data (No longer updated)More details  |

## First-Aid:

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| Eye: Irrigate immediately (liquid)/Frostbite Skin: Water flush immediately (liquid)/Frostbite Breathing: Respiratory supportNIOSHIP8750000  |

## Exposure Routes:

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| inhalation, skin and/or eye contact (liquid)NIOSHIP8750000  |

## Symptoms:

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| Irritation nose, throat; sneezing, cough, dyspnea (breathing difficulty); pulmonary edema; conjunctivitis; dermatitis; liquid: frostbiteNIOSHIP8750000  |

## Target Organs:

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| Eyes, skin, respiratory systemNIOSHIP8750000  |

## Incompatibility:

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| Strong oxidizers, chlorine, mercury, acraldehyde, fluorides, maleic anhydride, aluminum, brass, copper, zincNIOSHIP8750000  |

## Personal Protection:

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| --- |
| Skin: Prevent skin contact (liquid)/Frostbite Eyes: Prevent eye contact (liquid)/Frostbite Wash skin: When contaminated (liquid) Remove: When wet (flammable) Change: No recommendation Provide: Eyewash(liquid), Quick drench (liquid), Frostbite washNIOSHIP8750000  |

## Exposure Limits:

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| --- |
| NIOSH REL : TWA 10 ppm (18 mg/m 3 ) OSHA PEL : TWA 10 ppm (18 mg/m 3 )NIOSHIP8750000  |

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 419 (estimated with error: 83)NIST Spectramainlib\_291481, replib\_158546, replib\_229435  |
| 405 (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: 124403; 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.)NIST Spectranist ri  |
| 434 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 100 C; CAS no: 124403; 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  |
| 458 (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: 124403; 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.)NIST Spectranist ri  |
| 646 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 179 C; CAS no: 124403; 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  |
| 650 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 152 C; CAS no: 124403; 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):

|  |
| --- |
| 434 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 124403; 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  |
| 425 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; End T: 250 C; CAS no: 124403; Active phase: OV-101; Carrier gas: N2/He; Phase thickness: 0. 10 um; Data type: Normal alkane RI; Authors: Zenkevich, I. G., Experimentally measured retention indices., 2005.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 426 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 60 C; End T: 240 C; CAS no: 124403; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Flamini, G.; Luigi Cioni, P.; Morelli, I., Volatiles from leaves, fruits, and virgin oil from Olea europaea Cv. Olivastra Seggianese from Italy, J. Agric. Food Chem., 51, 2003, 1382-1386.)NIST Spectranist ri  |

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

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| --- | --- |
| Density:  | 0. 6±0. 1 g/cm 3  |
| Boiling Point:  | 6. 1±3. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 1520. 3±0. 0 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 26. 4±0. 0 kJ/mol  |
| Flash Point:  | -56. 1±8. 8 °C  |
| Index of Refraction:  | 1. 344  |
| Molar Refractivity:  | 14. 9±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 1  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | -0. 43  |
| ACD/LogD (pH 5. 5):  | -3. 38  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 1. 00  |
| ACD/LogD (pH 7. 4):  | -3. 18  |
| ACD/BCF (pH 7. 4):  | 1. 00  |
| ACD/KOC (pH 7. 4):  | 1. 00  |
| Polar Surface Area:  | 12 Å 2  |
| Polarizability:  | 5. 9±0. 5 10 -24 cm 3  |
| Surface Tension:  | 15. 5±3. 0 dyne/cm  |
| Molar Volume:  | 70. 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) = -0. 17Log Kow (Exper. database match) = -0. 38Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 16. 06 (Adapted Stein & Brown method)Melting Pt (deg C): -106. 24 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 47E+003 (Mean VP of Antoine & Grain methods)MP (exp database): -92. 2 deg CBP (exp database): 6. 8 deg CVP (exp database): 1. 52E+03 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1e+006log Kow used: -0. 38 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1. 63e+006 mg/L (40 deg C)Exper. Ref: SCHWEIZER, AE ET AL. (1978)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LWat Sol (Exper. database match) = 1630000. 00Exper. Ref: SCHWEIZER, AE ET AL. (1978)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 66E-005 atm-m3/moleGroup Method: 1. 81E-005 atm-m3/moleExper Database: 1. 77E-05 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 508E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -0. 38 (exp database)Log Kaw used: -3. 140 (exp database)Log Koa (KOAWIN v1. 10 estimate): 2. 760Log Koa (experimental database): 2. 000Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8799Biowin2 (Non-Linear Model) : 0. 9701Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 1240 (weeks )Biowin4 (Primary Survey Model) : 3. 8260 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6121Biowin6 (MITI Non-Linear Model): 0. 7268Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8542Ready 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. 03E+005 Pa (1. 52E+003 mm Hg)Log Koa (Exp database): 2. 000Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 48E-011 Octanol/air (Koa) model: 2. 45E-011 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 5. 35E-010 Mackay model : 1. 18E-009 Octanol/air (Koa) model: 1. 96E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 65. 5296 E-12 cm3/molecule-secHalf-Life = 0. 163 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 959 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 8. 59E-010 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 13. 4Log Koc: 1. 127 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. 500 (BCF = 3. 162)log Kow used: -0. 38 (expkow database)Volatilization from Water: Henry LC: 1. 77E-005 atm-m3/mole (Henry experimental database)Half-Life from Model River: 22. 89 hoursHalf-Life from Model Lake : 306. 1 hours (12. 75 days)Removal In Wastewater Treatment: Total removal: 2. 81 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 74 percentTotal to Air: 0. 98 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 712 3. 78 1000 Water 48. 9 360 1000 Soil 50. 3 720 1000 Sediment 0. 0898 3. 24e+003 0 Persistence Time: 304 hr

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