

# [2-aminopropane c3h9n structure](https://assignbuster.com/2-aminopropane-c3h9n-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula | C 3 H 9 N |
| Average mass | 59. 110 Da |
| Density | 0. 7±0. 1 g/cm 3 |
| Boiling Point | 30. 9±8. 0 °C at 760 mmHg |
| Flash Point | -32. 2±0. 0 °C |
| Molar Refractivity | 19. 4±0. 3 cm 3 |
| Polarizability | 7. 7±0. 5 10 -24 cm 3 |
| Surface Tension | 22. 0±3. 0 dyne/cm |
| Molar Volume | 82. 1±3. 0 cm 3 |

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

## Experimental Melting Point:

|  |
| --- |
| -101 °CAlfa Aesar |
| -95 °CJean-Claude Bradley Open Melting Point Dataset13115 |
| -95. 13 °CJean-Claude Bradley Open Melting Point Dataset21295 |
| -101 °CJean-Claude Bradley Open Melting Point Dataset7384 |
| -101 °CAlfa AesarA15044 |
| -101 °CLabNetworkLN00195372 |
| -95. 1 °CFooDBFDB009650 |

## Experimental Boiling Point:

|  |
| --- |
| 33-34 °CAlfa Aesar |
| 91 F (32. 7778 °C)NIOSHNT8400000 |
| 34 °CFood and Agriculture Organization of the United Nations2-Aminopropane |
| 32 °CArkema[ARK12],[ARK13] |
| 53 °CArkema[ARK12],[ARK13] |
| 33-34 °CAlfa AesarA15044 |
| 33-34 °COakwood094589 |
| 33-34 °CLabNetworkLN00195372 |

## Experimental Ionization Potent:

|  |
| --- |
| 8. 72 EvNIOSHNT8400000 |

## Experimental Vapor Pressure:

|  |
| --- |
| 460 mmHgNIOSHNT8400000 |

## Experimental Flash Point:

|  |
| --- |
| -32 °CAlfa Aesar |
| -32 °CAlfa Aesar |
| -32 °F (-35. 5556 °C)Alfa AesarA15044 |
| -18 °COakwood094589 |
| -20 °CLabNetworkLN00195372 |

## Experimental Freezing Point:

|  |
| --- |
| -150 F (-101. 1111 °C)NIOSHNT8400000 |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLMerck Millipore1750, 4487 |
| 0 g/mLArkema[ARK12],[ARK12],[ARK13],[ARK13] |
| 20 g/lMerck Millipore1750, 4487, 845053, 807476 |
| 0. 691 g/mLAlfa AesarA15044 |
| 0. 688 g/mLOakwood094589 |
| 0. 72 g/mLFluorochem094589 |
| 0. 69 g/lFluorochem094589 |

## Experimental Refraction Index:

|  |
| --- |
| 1. 3746Alfa AesarA15044 |
| 1. 367-1. 373Food and Agriculture Organization of the United Nations2-Aminopropane |

## Experimental Solubility:

|  |
| --- |
| MiscibleNIOSHNT8400000 |

* Miscellaneous

## Appearance:

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| --- |
| Colorless liquid with an ammonia-like odor. [Note: A gas above 91F.]NIOSHNT8400000 |
| Colourless to yellow liquid; Fishy ammonia aromaFood and Agriculture Organization of the United Nations2-Aminopropane |

## Safety:

|  |
| --- |
| 12-36/37/38Alfa AesarA15044 |
| 16-26-29Alfa AesarA15044 |
| 3Alfa AesarA15044 |
| DangerAlfa AesarA15044 |
| DANGER: FLAMMABLE, irritates skin and eyesAlfa AesarA15044 |
| DANGER: FLAMMABLE, POISON, CORROSIVE, irritantAlfa AesarA15044 |
| H224-H315-H319-H335Alfa AesarA15044 |
| P210-P261-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarA15044 |

## First-Aid:

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| Eye: Irrigate immediately Skin: Water flush immediately Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHNT8400000 |

## Exposure Routes:

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| --- |
| inhalation, skin absorption, ingestion, skin and/or eye contactNIOSHNT8400000 |

## Symptoms:

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| --- |
| Irritation eyes, skin, nose, throat; pulmonary edema; visual disturbance; eye, skin burns; dermatitisNIOSHNT8400000 |

## Target Organs:

|  |
| --- |
| Eyes, skin, respiratory systemNIOSHNT8400000 |

## Incompatibility:

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| --- |
| Strong acids, strong oxidizers, aldehydes, ketones, epoxidesNIOSHNT8400000 |

## Personal Protection:

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| --- |
| Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet (flammable) Change: No recommendation Provide: Eyewash, Quick drenchNIOSHNT8400000 |

## Exposure Limits:

|  |
| --- |
| NIOSH REL : See Appendix D OSHA PEL ?: TWA 5 ppm (12 mg/m 3 )NIOSHNT8400000 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 498 (estimated with error: 83)NIST Spectramainlib\_341956, replib\_154506, replib\_229257 |
| 469 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 1 m; Column type: Packed; Start T: 130 C; CAS no: 75310; Active phase: OV-101; Carrier gas: Ar; Substrate: Chromosorb W HP; Data type: Kovats RI; Authors: Osmialowski, K.; Halkiewicz, J.; Radecki, A.; Kaliszan, R., Quantum chemical parameters in correlation analysis of gas-liquid chromatographic retention indices of amines, J. Chromatogr., 346, 1985, 53-60.)NIST Spectranist ri |
| 468 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 75310; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb W AW; Data type: Kovats RI; Authors: Oszczapowicz, J.; Osek, J.; Dolecka, E., Retention indices of dimethylformamidines, dimethylacetamidines and tetramethylguanidines on a non-polar column, J. Chromatogr., 315, 1984, 95-100.)NIST Spectranist ri |
| 477 (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: 75310; Active phase: Apiezon L; Carrier gas: N2 or He; Substrate: Chromosorb G, AW; Data type: Kovats RI; Authors: Zhuravleva, I. L.; Kapustin, Yu. P.; Golovnya, P. B., Retention indices of some isoaliphatic and heterocyclic nitrogenous bases, Zh. Anal. Khim., 31, 1976, 1378-1380.)NIST Spectranist ri |
| 710 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 179 C; CAS no: 75310; 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 |
| 725 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 152 C; CAS no: 75310; 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 |
| 740 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 75310; 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., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 75310; 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 |
| 743 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 120 C; CAS no: 75310; 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):

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| --- |
| 465 (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: 75310; 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., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 75310; Active phase: Polydimethyl siloxanes; Data type: Normal alkane RI; Authors: Zenkevich, I. G.; Chupalov, A. A., New Possibilities of Chromato Mass Pectrometric Identification of Organic Compounds Using Increments of Gas Chromatographic Retention Indices of Molecular Structural Fragments, Zh. Org. Khim. (Rus.), 32(5), 1996, 656-666, In original 656-666.)NIST Spectranist ri |
| 469 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 130 C; CAS no: 75310; Active phase: OV-101; Data type: Normal alkane RI; Authors: Qi, Y.; Yang, J.; Xu, L., correlation analysis of the structures and gas liquid chromatographic retention indices of amines, Chin. J. Anal. Chem., 28(2), 2000, 223-227.)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: | 30. 9±8. 0 °C at 760 mmHg |
| Vapour Pressure: | 607. 7±0. 1 mmHg at 25°C |
| Enthalpy of Vaporization: | 27. 8±0. 0 kJ/mol |
| Flash Point: | -32. 2±0. 0 °C |
| Index of Refraction: | 1. 389 |
| Molar Refractivity: | 19. 4±0. 3 cm 3 |
| #H bond acceptors: | 1 |
| #H bond donors: | 2 |
| #Freely Rotating Bonds: | 0 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 0. 21 |
| ACD/LogD (pH 5. 5): | -2. 76 |
| ACD/BCF (pH 5. 5): | 1. 00 |
| ACD/KOC (pH 5. 5): | 1. 00 |
| ACD/LogD (pH 7. 4): | -2. 54 |
| ACD/BCF (pH 7. 4): | 1. 00 |
| ACD/KOC (pH 7. 4): | 1. 00 |
| Polar Surface Area: | 26 Å 2 |
| Polarizability: | 7. 7±0. 5 10 -24 cm 3 |
| Surface Tension: | 22. 0±3. 0 dyne/cm |
| Molar Volume: | 82. 1±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. 27Log Kow (Exper. database match) = 0. 26Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 47. 27 (Adapted Stein & Brown method)Melting Pt (deg C): -83. 69 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 592 (Mean VP of Antoine & Grain methods)MP (exp database): -95. 1 deg CBP (exp database): 31. 7 deg CVP (exp database): 5. 80E+02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 8. 381e+005log Kow used: 0. 26 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1e+006 mg/L (25 deg C)Exper. Ref: DORIGAN, J ET AL. (1976) @2NDWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 6. 5379e+005 mg/LWat Sol (Exper. database match) = 1000000. 00Exper. Ref: DORIGAN, J ET AL. (1976) @2NDECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 34E-005 atm-m3/moleGroup Method: IncompleteExper Database: 4. 51E-05 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 5. 494E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 26 (exp database)Log Kaw used: -2. 734 (exp database)Log Koa (KOAWIN v1. 10 estimate): 2. 994Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8732Biowin2 (Non-Linear Model) : 0. 9637Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0930 (weeks )Biowin4 (Primary Survey Model) : 3. 8057 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5197Biowin6 (MITI Non-Linear Model): 0. 6163Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 6884Ready 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): 7. 73E+004 Pa (580 mm Hg)Log Koa (Koawin est ): 2. 994Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 88E-011 Octanol/air (Koa) model: 2. 42E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 4E-009 Mackay model : 3. 1E-009 Octanol/air (Koa) model: 1. 94E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 39. 3766 E-12 cm3/molecule-secHalf-Life = 0. 272 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 260 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 25E-009 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 26. 32Log Koc: 1. 420 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. 26 (expkow database)Volatilization from Water: Henry LC: 4. 51E-005 atm-m3/mole (Henry experimental database)Half-Life from Model River: 10. 77 hoursHalf-Life from Model Lake : 181. 9 hours (7. 579 days)Removal In Wastewater Treatment: Total removal: 4. 19 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 73 percentTotal to Air: 2. 38 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 1. 52 6. 52 1000 Water 48. 9 360 1000 Soil 49. 5 720 1000 Sediment 0. 091 3. 24e+003 0 Persistence Time: 272 hr

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