

# [Niacin c6h5no2 structure](https://assignbuster.com/niacin-c6h5no2-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 6 H 5 NO 2  |
| Average mass  | 123. 109 Da  |
| Density  | 1. 3±0. 1 g/cm 3  |
| Boiling Point  | 292. 5±13. 0 °C at 760 mmHg  |
| Flash Point  | 130. 7±19. 8 °C  |
| Molar Refractivity  | 31. 3±0. 3 cm 3  |
| Polarizability  | 12. 4±0. 5 10 -24 cm 3  |
| Surface Tension  | 58. 8±3. 0 dyne/cm  |
| Molar Volume  | 95. 2±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 236-239 °C (Sublimes)SynQuest  |
| 238 °CTCIN0082  |
| 236-239 °CAlfa Aesar  |
| 237 °COxford University Chemical Safety Data (No longer updated)More details  |
| 236. 6 °CLKT Labs[N3301]  |
| 234-238 °CMerck Millipore2882, 818714  |
| 237 °CJean-Claude Bradley Open Melting Point Dataset15999, 16664  |
| 236. 6 °CJean-Claude Bradley Open Melting Point Dataset17322, 22338, 28307, 28308, 28309  |
| 238 °CJean-Claude Bradley Open Melting Point Dataset8079  |
| 236-239 °CAlfa AesarA12683  |
| 236-239 °C (Sublimes)SynQuest60871, 4H56-1-4A  |
| 236-239 °COakwood214893  |
| 236-239 °C (Literature)LabNetwork  |
| 236-239 °CLabNetworkLN00180010  |
| 236-239 °CIndofine[BIO-301]  |

## Experimental LogP:

|  |
| --- |
| 0. 147Vitas-MSTK301803  |

## Experimental Flash Point:

|  |
| --- |
| 293 °CAlfa Aesar  |
| 293 °CAlfa Aesar  |
| 293 °F (145 °C)Alfa AesarA12683  |
| 193 °CSynQuest60871, 4H56-1-4A  |
| 193 °COakwood214893  |
| 193 °CLabNetworkLN00180010  |

## Experimental Gravity:

|  |
| --- |
| 1. 4 g/mLAlfa AesarA12683  |
| 1. 47 g/mLSynQuest4H56-1-4A  |

## Experimental Solubility:

|  |
| --- |
| 10 mM in H2OMedChem ExpressHY-B0143  |
| water: 15 g/l (at 20 °C); hot alcohol, alkali hydroxides, propylene glycolMedChem ExpressHY-B0143  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 238 °CTCI  |
| 238 °CTCIN0082  |

* Miscellaneous

## Appearance:

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| --- |
| white crystalline powderOxford University Chemical Safety Data (No longer updated)More details  |
| WHITE POWDERNIH Clinical Collection[SMR000059024]  |

## Stability:

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 Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 7000 mg kg-1, IPR-RAT LD50 730 mg kg-1, SCU-RAT LD50 5000 mg kg-1, ORL-MUS LD50 5000 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 26Alfa AesarA12683  |
| 26-60Alfa AesarA12683  |
| 36Alfa AesarA12683  |
| H319Alfa AesarA12683  |
| H330, H319, H311, H301LKT Labs[N3301]  |
| IRRITANTMatrix Scientific082487  |
| Irritant/Light Sensitive/Store under ArgonSynQuest4H56-1-4A, 60871  |
| None. Oxford University Chemical Safety Data (No longer updated)More details  |
| P280-P264-P305+P351+P338-P337+P313Alfa AesarA12683  |
| R26-36-24/25LKT Labs[N3301]  |
| T+, Xi, TLKT Labs[N3301]  |
| WarningAlfa AesarA12683  |
| WARNING: Not for human consumption, may irriate skin & eyes. Alfa AesarA12683  |
| WARNING: Not sold for human treatment, trials or useAlfa AesarA12683  |
| XiAbblis ChemicalsAB1002056  |

## Target Organs:

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| --- |
| VBTargetMolT0879  |

## Chemical Class:

|  |
| --- |
| alkaloidMicrosource[01500430]  |

## Compound Source:

|  |
| --- |
| widespread in the plant and fungal kingdomMicrosource[01500430]  |

## Bio Activity:

|  |
| --- |
| Niacin (Vitamin B3) is a water-soluble vitamin and is part of the vitamin B group. MedChem Express  |
| Niacin (Vitamin B3) is a water-soluble vitamin and is part of the vitamin B group.; Target: Others; Niacin (also known as vitamin B3 and nicotinic acid) is an organic compound with the formula C6H5NO2 and, depending on the definition used, one of the 20 to 80 essential human nutrients. MedChem ExpressHY-B0143  |
| Niacin (Vitamin B3) is a water-soluble vitamin and is part of the vitamin B group.; Target: Niacin (also known as vitamin B3 and nicotinic acid) is an organic compound with the formula C6H5NO2 and, depending on the definition used, one of the 20 to 80 essential human nutrients. Not enough niacin in the diet can cause nausea, skin and mouth lesions, anemia, headaches, and tiredness. Chronic Niacin deficiency leads to a disease called pellagra. The lack of niacin may also be observed in pandemic deficiency disease which is caused by a lack of five crucial vitamins: niacin, vitamin C, thiamin, vitamin D and vitamin A, and is usually found in areas of widespread poverty and malnutrition. Niacin has been used for over 50 years to increase levels of HDL in the blood and has been found to decrease the risk of cardiovascular events modestly in a number of controlled human trials. Niacin cannot be directly converted to nicotinamide, but both compounds could be converted to and are precMedChem ExpressHY-B0143  |
| OthersMedChem ExpressHY-B0143  |
| VB3TargetMolT0879  |
| VitaminTargetMolT0879  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1144 (estimated with error: 89)NIST Spectramainlib\_233225, replib\_312948, replib\_155087, replib\_291061, replib\_379751  |
| 1340 (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: 130 C; CAS no: 59676; Active phase: DB-1; Carrier gas: N2; Phase thickness: 1. 5 um; Data type: Kovats RI; Authors: Japp, M.; Gill, R.; Osselton, M. D., Comparison of drug retention indices determined on packed, wide bore capillary and narrow bore capillary columns, J. Forensic Sci., 32(6), 1987, 1574-1586.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1335 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Other; CAS no: 59676; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 1335 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 1. 8 m; Column type: Packed; Heat rate: 8 K/min; Start T: 130 C; End T: 290 C; End time: 8 min; Start time: 2 min; CAS no: 59676; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb W; Data type: Linear RI; Authors: Perrigo, B. J.; Peel, H. W., The use of retention indices and temperature-programmed gas chromatography in analytical toxicology, J. Chromatogr. Sci., 19, 1981, 219-226.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 1. 3±0. 1 g/cm 3  |
| Boiling Point:  | 292. 5±13. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 6 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 56. 2±3. 0 kJ/mol  |
| Flash Point:  | 130. 7±19. 8 °C  |
| Index of Refraction:  | 1. 571  |
| Molar Refractivity:  | 31. 3±0. 3 cm 3  |
| #H bond acceptors:  | 3  |
| #H bond donors:  | 1  |
| #Freely Rotating Bonds:  | 1  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 0. 15  |
| ACD/LogD (pH 5. 5):  | -1. 54  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 1. 00  |
| ACD/LogD (pH 7. 4):  | -2. 60  |
| ACD/BCF (pH 7. 4):  | 1. 00  |
| ACD/KOC (pH 7. 4):  | 1. 00  |
| Polar Surface Area:  | 50 Å 2  |
| Polarizability:  | 12. 4±0. 5 10 -24 cm 3  |
| Surface Tension:  | 58. 8±3. 0 dyne/cm  |
| Molar Volume:  | 95. 2±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. 69Log Kow (Exper. database match) = 0. 36Exper. Ref: Sangster (1993)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 257. 62 (Adapted Stein & Brown method)Melting Pt (deg C): 63. 27 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 9. 36E-005 (Modified Grain method)MP (exp database): 236. 6 deg CSubcooled liquid VP: 0. 018 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): 4. 815e+004log Kow used: 0. 36 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1. 8e+004 mg/L (25 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 9678. 1 mg/LWat Sol (Exper. database match) = 18000. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral Organics-acidHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 42E-010 atm-m3/moleGroup Method: 5. 11E-011 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 3. 149E-010 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 36 (exp database)Log Kaw used: -8. 236 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 8. 596Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7112Biowin2 (Non-Linear Model) : 0. 8854Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8008 (weeks )Biowin4 (Primary Survey Model) : 3. 6591 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 7222Biowin6 (MITI Non-Linear Model): 0. 8080Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 3610Ready 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. 4 Pa (0. 018 mm Hg)Log Koa (Koawin est ): 8. 596Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 25E-006 Octanol/air (Koa) model: 9. 68E-005 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 4. 51E-005 Mackay model : 0. 0001 Octanol/air (Koa) model: 0. 00769 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 6570 E-12 cm3/molecule-secHalf-Life = 16. 280 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 7. 26E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 14. 49Log Koc: 1. 161 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. 36 (expkow database)Volatilization from Water: Henry LC: 5. 11E-011 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 271E+007 hours (5. 297E+005 days)Half-Life from Model Lake : 1. 387E+008 hours (5. 779E+006 days)Removal In Wastewater Treatment: Total removal: 1. 86 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 00119 391 1000 Water 37. 8 360 1000 Soil 62. 1 720 1000 Sediment 0. 0707 3. 24e+003 0 Persistence Time: 587 hr

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* 1-Click Scaffold Hop