Niacin c6h5no2 structure

ASSIGN BUSTER

Contents

- Retention Index (Linear):

Molecular Formula	$C_6H_5NO_2$
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237 °COxford University Chemical Safety Data (No longer updated)More details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 glycolM

  ExpressHY-B0143

- Predicted Physico-chemical Properties

  - **Predicted Melting Point:**

    238 °CTCI

    238

    °CTCIN0082

- Miscellaneous

  - **Appearance:**

    white crystalline powderOxford University Chemical Safety Data (No long

    updated)More details

    WHITE POWDERNIH Clinical Collection[SMR000059024]

  - **Stability:**

    Stable. Incompatible with strong oxidizing agents. May belight sensitive.

    University Chemical Safety Data (No longer updated)More details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

  mg kg-1, ORL-MUS LD50 5000 mg kg-1Oxford University Chemical Safety

  (No longer updated)More details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:**

VBTargetMolT087

9

- **Chemical Class:**

alkaloidMicrosource[0150

0430]

- **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

MedChem Express

Niacin (Vitamin B3) is a water-soluble vitamin and is part of the vitamin B

Target: Others; Niacin (also known as vitamin B3 and nicotinic acid) is an
compound with the formula C6H5NO2 and, depending on the definition u
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
Target: Niacin (also known as vitamin B3 and nicotinic acid) is an organic
compound with the formula C6H5NO2 and, depending on the definition u
of the 20 to 80 essential human nutrients. Not enough niacin in the diet c
cause nausea, skin and mouth lesions, anemia, headaches, and tiredness
Chronic Niacin deficiency leads to a disease called pellagra. The lack of n
may also be observed in pandemic deficiency disease which is caused by
of five crucial vitamins: niacin, vitamin C, thiamin, vitamin D and vitamin
is usually found in areas of widespread poverty and malnutrition. Niacin h
used for over 50 years to increase levels of HDL in the blood and has bee
to decrease the risk of cardiovascular events modestly in a number of co
human trials. Niacin cannot be directly converted to nicotinamide, but bo
compounds could be converted to and are precMedChem ExpressHY-B01

OthersMedChem ExpressHY-B0143

VB3TargetMolT0879

VitaminTargetMolT0879

- Gas Chromatography

- **Retention Index (Kovats):**

  1144 (estimated with error: 89)NIST Spectramainlib_233225, replib_3129

replib_155087, replib_291061, replib_379751

1340 (Program type: Isothermal; Col... (show more)umn class: Standard polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: C Start T: 130 C; CAS no: 59676; Active phase: DB-1; Carrier gas: N2; Phas thickness: 1. 5 um; Data type: Kovats RI; Authors: Japp, M.; Gill, R.; Ossel D., Comparison of drug retention indices determined on packed, wide bo capillary and narrow bore capillary columns, J. Forensic Sci., 32(6), 1987, 1586.)NIST Spectranist ri

- **Retention Index (Normal Alkane):**

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

- **Retention Index (Linear):**

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

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

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop