Nicorandil c8h9n3o4 structure

Contents

Molecular Formula	$C_8H_9N_3O_4$
Average mass	211. 175 Da
Density	1. 3±0. 1 g/cm ^{3}
Boiling Point	456. 7±25. 0 °C at 760 mmHg
Flash Point	230. 0±23. 2 °C
Molar Refractivity	50. 4±0. 3 cm ^{3}
Polarizability	20. 0±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	55. 3±3. 0 dyne/cm
Molar Volume	158. 7±3. 0 cm ^{3}

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

Experimental Melting Point:

90 °CTCIN0837

92. 5 °CJean-Claude

Bradley Open Melting

Point Dataset22728

92-93

°CLabNetworkLN00222

789

Experimental Flash Point:

230

°CLabNetworkLN00222789

Experimental Solubility:

DMSO 40 mg/mL;

Water 17

mg/mLMedChem

ExpressHY-B0341

DMSO:

25mg/mLMedChem

ExpressHY-B0341

Soluble to 20 mM in

waterTocris

Bioscience2147

- Predicted Physico-chemical Properties

  - **Predicted Melting Point:**

    90 °CTCI

    90

    °CTCIN0837

- Miscellaneous

  - **Target Organs:**

    Potassium Channel

    activatorTargetMolT00

    75

  - **Drug Status:**

    approvedBIONET-Key OrganicsHS-

    0049

  - **Bio Activity:**

    Antioxidant; Zerenex

    Molecular[ZBioX-0564]

Inward rectifier

Potassium

ChannelsTocris

Bioscience2147

Ion ChannelsTocris

Bioscience2147

Kir6 (KATP) channel

opener and NO

donorTocris

Bioscience2147

Kir6 (KATP) channel

opener and NO donor;

antianginal agent.

Preferentially activates

SUR2B- versus SUR2A-

containing Kir6

channels (EC50 values

are 10 and > 500 ? M

respectively) and

causes 1. 6-fold

increase in cardiac

eNOS expression.

Displays coronary and

peripheral vasodilatory

properties, reduces both pre- and after-load, and increases coronary blood flow. Also displays cardioprotective effects, possibly through ischemic preconditioning. Tocris Bioscience2147

Kir6 (KATP) channel opener and NO donor; antianginal agent. Preferentially activates SUR2B- versus SUR2A-containing Kir6 channels (EC50 values are 10 and > 500 ? M respectively) and causes 1. 6-fold increase in cardiac eNOS expression. Displays coronary and peripheral vasodilatory properties, reduces

both pre- and after-

load, and increases

coronary blood flow.

Also displays

cardioprotective

effects, possibly

through ischemic

preconditioning. Tocris

Bioscience2147

Membrane

Tranporter/Ion

ChannelMedChem

ExpressHY-B0341

Membrane

Tranporter/Ion

Channel; MedChem

ExpressHY-B0341

Membrane

Transporter/Ion

ChannelTargetMolT007

5

Nicorandil is potassium

channel activator.

MedChem Express

Nicorandil is potassium channel activator.; Target: Potassium Channel; Nicorandil is a vasodilatory drug used to treat angina.

MedChem ExpressHY-B0341

Nicorandil is potassium channel activator.; Target: Potassium ChannelNicorandil is a vasodilatory drug used to treat angina.

Nicorandil stimulates guanylate cyclase to increase formation of cyclic GMP (cGMP). cGMP activates protein kinase G (PKG) which phosphorylates and inhibits GTPase RhoA and decreases Rho-

kinase activity.

Reduced Rho-kinase activity permits an increase in myosin phosphatase activity, decreasing the calcium sensitivity of the smooth muscle. PKG also activates the sarcolemma calcium pump to remove activating calcium. PKG acts on K+ channels to promote K+ efflux and the ensuing hyperpolarization inhibits voltage-gated calcium channels. Overall, this leads to relaxation of the smooth muscle and coronary vasodilation [1, 2]. MedChem ExpressHY-B0341

Potassium

ChannelTargetMolT007

5

Potassium

ChannelsTocris

Bioscience2147

Potassiun

ChannelMedChem

ExpressHY-B0341

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

Density:	1. 3±0. 1 g/cm ^{3}
Boiling Point:	456. 7±25. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 1 mmHg at 25°C
Enthalpy of Vaporization:	71. 7±3. 0 kJ/mol
Flash Point:	230. 0±23. 2 °C
Index of Refraction:	1. 548
Molar Refractivity:	50. 4±0. 3 cm ^{3}
#H bond acceptors:	7
#H bond donors:	1

#Freely Rotating Bonds:	5
#Rule of 5 Violations:	0
ACD/LogP:	0. 72
ACD/LogD (pH 5. 5):	0. 93
ACD/BCF (pH 5. 5):	2. 97
ACD/KOC (pH 5. 5):	75. 69
ACD/LogD (pH 7. 4):	0. 93
ACD/BCF (pH 7. 4):	2. 99
ACD/KOC (pH 7. 4):	76. 16
Polar Surface Area:	97 Å ^{2}
Polarizability:	20. 0±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	55. 3±3. 0 dyne/cm
Molar Volume:	158. 7±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. 43Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 376. 76 (Adapted Stein & Brown method)Melting Pt (deg C): 143. 02 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 6. 76E-006 (Modified Grain method)MP (exp database): 92. 5 deg CSubcooled liquid VP: 3. 03E-005 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): 1. 643e+004log Kow used: 0. 43 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3. 9664e+005 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 28E-014 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 143E-010 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 43 (KowWin est)Log Kaw used: -12. 031 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 12. 461Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7026Biowin2 (Non-Linear Model) : 0. 7433Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 4641 (weeks-months)Biowin4 (Primary Survey Model) : 3. 7297 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3087Biowin6 (MITI Non-Linear Model): 0. 1412Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 5795Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 00404 Pa (3. 03E-005 mm Hg)Log Koa (Koawin est): 12. 461Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 000743 Octanol/air (Koa) model: 0. 71 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0261 Mackay model : 0. 0561 Octanol/air (Koa) model: 0. 983 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 1. 5091 E-12 cm3/molecule-secHalf-Life = 7. 088 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 85. 051 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 0411 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 254. 6Log Koc: 2. 406 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. 43 (estimated)Volatilization from Water: Henry LC: 2. 28E-014 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 3. 732E+010 hours (1. 555E+009 days)Half-Life from Model Lake : 4. 071E+011 hours (1. 696E+010 days)Removal In Wastewater Treatment: Total removal: 1. 86 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 77 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 3. 15e-007 170 1000 Water 44. 7 900 1000 Soil 55. 2 1. 8e+003 1000 Sediment 0. 088 8. 1e+003 0 Persistence Time: 996 hr

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- 1-Click Docking
- 1-Click Scaffold Hop