Pantoprazole c16h15f2n3o4s structure

Contents

Molecular Formula	$C_{16}H_{15}F_2N_3O_4S$
Average mass	383. 370 Da
Density	1. 5±0. 1 g/cm ^{3}
Boiling Point	586. 9±60. 0 °C at 760 mmHg
Flash Point	308. 7±32. 9 °C
Molar Refractivity	91. 4±0. 4 cm ^{3}
Polarizability	36. 2±0. 5 10^{-24} cm ^{3}
Surface Tension	73. 5±5. 0 dyne/cm
Molar	252. 7±5. 0

Volume cm^3

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

Experimental Melting Point:

139 °C

(Decomposes)L

KT Labs[P0255]

Experimental Solubility:

10 mM in DMSO;

in

MethanolMedCh

em ExpressHY-

17507

DMSO:

45mg/mLMedCh

em ExpressHY-

17507

Soluble in

methanol. LKT

Labs[P0255]

- Miscellaneous

Safety:

H302LKT

Labs[P0255]

Compound Source:

synthetic; SK&F-

96022, BY-

1023Microsourc

e[01505818]

Bio Activity:

Membrane

Tranporter/Ion

ChannelMedChe

m ExpressHY-

17507

Membrane

Tranporter/Ion

Channel;

MedChem

ExpressHY-

17507

Pantoprazole(SK F96022; Protonix) is a proton pump inhibitor drug used for short-term treatment of erosion and ulceration of the esophagus caused by gastroesophageal reflux disease. MedChem Express

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Pantoprazole(SKF96022; Protonix) is a proton pump inhibitor drug used for short-term treatment of erosion and ulceration of the esophagus caused by gastroesophageal reflux

	disease.; IC50 value:; Target: proton pump inhibitorMedChem ExpressHY-17507
	Proton PumpMedChem ExpressHY-17507

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

Density:	1. 5±0. 1 g/cm ^{3}
Boiling Point:	586. 9±60. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 6 mmHg at 25°C
Enthalpy of Vaporization:	87. 6±3. 0 kJ/mol
Flash Point:	308. 7±32. 9 °C
Index of Refraction:	1. 643
Molar Refractivity:	91. 4±0. 4 cm ^{3}
#H bond acceptors:	7

#H bond donors:	1
#Freely Rotating Bonds:	7
#Rule of 5 Violations:	0
ACD/LogP:	1. 69
ACD/LogD (pH 5. 5):	1. 45
ACD/BCF (pH 5. 5):	7. 49
ACD/KOC (pH 5. 5):	146. 78
ACD/LogD (pH 7. 4):	1. 45
ACD/BCF (pH 7. 4):	7. 35
ACD/KOC (pH 7. 4):	144. 15
Polar Surface Area:	106 Å ^{2}
Polarizability:	36. 2±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	73. 5±5. 0 dyne/cm
Molar Volume:	252. 7±5. 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) = 2. 22Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 575. 10 (Adapted Stein & Brown method)Melting Pt (deg C): 247. 68 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 25E-012 (Modified Grain method)Subcooled liquid VP: 3. 28E-010 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): 48. 84log Kow used: 2. 22 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 25360 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: ImidazolesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 84E-020 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 291E-014 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 22 (KowWin est)Log Kaw used: -17. 622 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 19. 842Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8062Biowin2 (Non-Linear Model) : 0. 9353Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 1. 9634 (months)Biowin4 (Primary Survey Model) : 3. 5072 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 0941Biowin6 (MITI Non-Linear Model): 0. 0000Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 2017Ready 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): 4. 37E-008 Pa (3. 28E-010 mm Hg)Log Koa (Koawin est): 19. 842Kp (particle/gas partition coef. (m3/ug)): Mackay model : 68. 6 Octanol/air (Koa) model: 1. 71E+007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1 Mackay model : 1 Octanol/air (Koa) model: 1 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 101. 5921 E-12 cm3/molecule-secHalf-Life = 0. 105 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 263 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 1 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 333E+004Log Koc: 4. 125 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 = 1. 013 (BCF = 10. 3)log Kow used: 2. 22 (estimated)Volatilization from Water: Henry LC: 5. 84E-020 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 963E+016 hours (8. 179E+014 days)Half-Life from Model Lake : 2. 141E+017 hours (8. 923E+015 days)Removal In Wastewater Treatment: Total removal: 2. 51 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 41 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 1. 71e-009 2. 53 1000 Water 18. 8 1. 44e+003 1000 Soil 81. 1 2. 88e+003 1000 Sediment 0. 1 1. 3e+004 0 Persistence Time: 2. 11e+003 hr

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