

# [Pantoprazole c16h15f2n3o4s structure](https://assignbuster.com/pantoprazole-c16h15f2n3o4s-structure/)

Contents

* Bio Activity:

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| --- | --- |
| Molecular Formula | C 16 H 15 F 2 N 3 O 4 S |
| 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 Volume | 252. 7±5. 0 cm 3 |

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

## Experimental Melting Point:

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| 139 °C (Decomposes)LKT Labs[P0255] |

## Experimental Solubility:

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| 10 mM in DMSO; in MethanolMedChem ExpressHY-17507 |
| DMSO: 45mg/mLMedChem ExpressHY-17507 |
| Soluble in methanol. LKT Labs[P0255] |

* Miscellaneous

## Safety:

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| H302LKT Labs[P0255] |

## Compound Source:

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| synthetic; SK&F-96022, BY-1023Microsource[01505818] |

## Bio Activity:

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| Membrane Tranporter/Ion ChannelMedChem ExpressHY-17507 |
| Membrane Tranporter/Ion Channel; MedChem ExpressHY-17507 |
| 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. MedChem Express |
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| Proton PumpMedChem ExpressHY-17507 |

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

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| --- | --- |
| 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 |

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| 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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