

Intepirdine  
c19h19n3o2s  
structure



## Contents

- Bio Activity:

Molecular  
Formula             $C_{19}H_{19}N_3O_2S$

Average mass 353.438 Da

Density             $1.3 \pm 0.1 \text{ g/cm}^3$

Boiling Point      $608.3 \pm 45.0 \text{ }^\circ\text{C}$  at  
760 mmHg

Flash Point        $321.7 \pm 28.7 \text{ }^\circ\text{C}$

Molar  
Refractivity        $99.6 \pm 0.4 \text{ cm}^3$

Polarizability     $39.5 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$

Surface  
Tension             $54.0 \pm 3.0 \text{ dyne/cm}$

Molar Volume     $273.4 \pm 3.0 \text{ cm}^3$

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite

- Predicted - ChemAxon
- Experimental Physico-chemical Properties

- **Experimental Solubility:**

10 mM in

DMSOMedChem

ExpressHY-14339

DMSO 78 mg/mL; Water

<1 mg/mLMedChem

Express[http://www.](http://www.medchemexpress.com/MK-5046.html)

medchemexpress.

com/MK-5046.html, HY-

14339

- Miscellaneous

- **Target Organs:**

5-HT Receptor

antagonistTargetMolT1774

- **Bio Activity:**

5-HT ReceptorMedChem

ExpressHY-14339

5-HT6TargetMolT1774

GPCR/G

proteinMedChem

ExpressHY-14339

GPCR/G protein;

Neuronal Signaling;

MedChem ExpressHY-

14339

NeuroscienceTargetMOLT

1774

SB742457 is a highly

selective 5-HT6 receptor

antagonist with pKi of 9.

63; exhibitsMedChem

Express[http://www.](http://www.medchemexpress.com/MK-5046.html)

medchemexpress.

com/MK-5046. html

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HT6 Receptor; SB-

742457, a 5-HT6  
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ExpressHY-14339

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this mechanistic approach. Alzheimer's disease is a devastating neurological condition characterized by a progressive decline in cognitive performance accompanied by behavioral and psychological syndromes, such as depression and psychosis. With the subsequent development of selective 5-HT6 receptor antagonists, preclinical studies in rodents and primates have elucidated the function of this receptor subtype in more detail. It is increasingly clear that blockade of 5-HT6 receptors leads to an improvement of

cognitive performance in  
a wide variety of  
learning and memory  
paradigms and also  
results in anxiolytic and  
antidepressant-like  
activity. SB-742457 is  
generally safe and  
weMedChem ExpressHY-  
14339

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

Density:	1.3 ± 0.1 g/cm <sup>3</sup>
Boiling Point:	608.3 ± 45.0 °C at 760 mmHg
Vapour Pressure:	0.0 ± 1.7 mmHg at 25°C
Enthalpy of Vaporization:	90.4 ± 3.0 kJ/mol
Flash Point:	321.7 ± 28.7 °C
Index of Refraction:	1.649
Molar Refractivity:	99.6 ± 0.4 cm <sup>3</sup>
#H bond acceptors:	5

#H bond donors:	1
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	2.10
ACD/LogD (pH 5.5):	-0.41
ACD/BCF (pH 5.5):	1.00
ACD/KOC (pH 5.5):	1.00
ACD/LogD (pH 7.4):	1.19
ACD/BCF (pH 7.4):	2.50
ACD/KOC (pH 7.4):	31.20
Polar Surface Area:	71 Å <sup>2</sup>
Polarizability:	39.5±0.5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	54.0±3.0 dyne/cm
Molar Volume:	273.4±3.0 cm <sup>3</sup>

Predicted data is generated using the US Environmental Protection Agency's EPISuite™

<https://assignbuster.com/intepirdine-c19h19n3o2s-structure/>



Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 3. 11Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 528. 01 (Adapted Stein & Brown method)Melting Pt (deg C): 225. 68 (Mean or Weighted MP)VP (mm Hg, 25 deg C): 3. 76E-011 (Modified Grain method)Subcooled liquid VP: 5. 33E-009 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): 133. 4log Kow used: 3. 11 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3769. 2 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenry's Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 69E-017 atm-m<sup>3</sup>/moleGroup Method: IncompleteHenry's LC [VP/WSol estimate using EPI values]: 1. 311E-013 atm-m<sup>3</sup>/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 11 (KowWin est)Log Kaw used: -14. 563 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 17. 673Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6559Biowin2 (Non-Linear Model) : 0. 2101Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 2098 (months )Biowin4 (Primary Survey Model) : 3. 0980 (weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 2298Biowin6 (MITI Non-Linear Model): 0. 0013Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -1. 2777Ready 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): 7. 11E-007 Pa (5. 33E-009 mm Hg)Log Koa (Koawin est ): 17. 673Kp (particle/gas partition coef. (m<sup>3</sup>/ug)): Mackay model : 4. 22 Octanol/air (Koa) model: 1. 16E+005 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 993 Mackay model : 0. 997 Octanol/air (Koa) model: 1 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 133. 6736 E-12 cm<sup>3</sup>/mole-secHalf-Life = 0. 080 Days (12-hr day; 1. 5E6 OH/cm<sup>3</sup>)Half-Life = 0. 960 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 995 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 3. 96E+005Log Koc: 5. 598 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. 693 (BCF = 49. 32)log Kow used: 3. 11 (estimated)Volatilization from Water: Henry LC: 6. 69E-017 atm-m<sup>3</sup>/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 645E+013 hours (6. 855E+011 days)Half-Life from Model Lake : 1. 795E+014 hours (7. 479E+012 days)Removal In Wastewater Treatment: Total removal: 6. 74 percentTotal biodegradation: 0. 13 percentTotal sludge adsorption: 6. 61 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 8. 34e-008 1. 92 1000 Water 10. 2 1. 44e+003 1000 Soil 89. 4 2. 88e+003 1000 Sediment 0. 334 1. 3e+004 0 Persistence Time: 2. 72e+003 hr

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