

# [Intepirdine c19h19n3o2s structure](https://assignbuster.com/intepirdine-c19h19n3o2s-structure/)

Contents

* Bio Activity:

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| --- | --- |
| Molecular Formula  | C 19 H 19 N 3 O 2 S  |
| Average mass  | 353. 438 Da  |
| Density  | 1. 3±0. 1 g/cm 3  |
| Boiling Point  | 608. 3±45. 0 °C at 760 mmHg  |
| Flash Point  | 321. 7±28. 7 °C  |
| Molar Refractivity  | 99. 6±0. 4 cm 3  |
| Polarizability  | 39. 5±0. 5 10 -24 cm 3  |
| Surface Tension  | 54. 0±3. 0 dyne/cm  |
| Molar Volume  | 273. 4±3. 0 cm 3  |

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

## Experimental Solubility:

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| --- |
| 10 mM in DMSOMedChem ExpressHY-14339  |
| DMSO 78 mg/mL; Water <1 mg/mLMedChem Expresshttp://www. medchemexpress. com/MK-5046. html, HY-14339  |

* Miscellaneous

## Target Organs:

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| 5-HT Receptor antagonistTargetMolT1774  |

## Bio Activity:

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| 5-HT ReceptorMedChem ExpressHY-14339  |
| 5-HT6TargetMolT1774  |
| GPCR/G proteinMedChem ExpressHY-14339  |
| GPCR/G protein; Neuronal Signaling; MedChem ExpressHY-14339  |
| NeuroscienceTargetMolT1774  |
| SB742457 is a highly selective 5-HT6 receptor antagonist with pKi of 9. 63; exhibitsMedChem Expresshttp://www. medchemexpress. com/MK-5046. html  |
| SB742457 is a highly selective 5-HT6 receptor antagonist with pKi of 9. 63; exhibits > 100-fold selectivity over other receptors.; IC50 Value: 9. 63 (pKi); Target: 5-HT6 Receptor; SB-742457, a 5-HT6 receptor antagonist, which extends into Alzheimer disease (AD) sufferers further highlights the therapeutic promise of this mechanistic approach. MedChem ExpressHY-14339  |
| SB742457 is a highly selective 5-HT6 receptor antagonist with pKi of 9. 63; exhibits > 100-fold selectivity over other receptors.; IC50 Value: 9. 63 (pKi); Target: 5-HT6 ReceptorSB-742457, a 5-HT6 receptor antagonist, which extends into Alzheimer disease (AD) sufferers further highlights the therapeutic promise of 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

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| --- | --- |
| Density:  | 1. 3±0. 1 g/cm 3  |
| 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 3  |
| #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 2  |
| Polarizability:  | 39. 5±0. 5 10 -24 cm 3  |
| Surface Tension:  | 54. 0±3. 0 dyne/cm  |
| Molar Volume:  | 273. 4±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) = 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 AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 69E-017 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 311E-013 atm-m3/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. (m3/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 cm3/molecule-secHalf-Life = 0. 080 Days (12-hr day; 1. 5E6 OH/cm3)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-m3/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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