

# [Harmine c13h12n2o structure](https://assignbuster.com/harmine-c13h12n2o-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula | C 13 H 12 N 2 O |
| Average mass | 212. 247 Da |
| Density | 1. 3±0. 1 g/cm 3 |
| Boiling Point | 421. 4±40. 0 °C at 760 mmHg |
| Flash Point | 139. 8±17. 0 °C |
| Molar Refractivity | 66. 0±0. 3 cm 3 |
| Polarizability | 26. 2±0. 5 10 -24 cm 3 |
| Surface Tension | 55. 7±3. 0 dyne/cm |
| Molar Volume | 169. 5±3. 0 cm 3 |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Predicted – Mcule
* Spectroscopy

## Lambda Max:

|  |
| --- |
| 338FooDBFDB002149 |

* Experimental Physico-chemical Properties

## Experimental Melting Point:

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| --- |
| 273 °CJean-Claude Bradley Open Melting Point Dataset25577 |
| 264 °CJean-Claude Bradley Open Melting Point Dataset7277 |
| 262-266 °CAlfa AesarL19068 |
| 266 °CBiosynthH-1200 |
| 230 °C (Decomposes)LabNetworkLN01307236 |
| 262-264 °CIndofine[H-005] |
| 264-265 °C / 257 mmHgFooDBFDB002149 |

## Experimental LogP:

|  |
| --- |
| 3. 173Vitas-MSTK047386 |

## Experimental Solubility:

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| --- |
| Soluble to 100 mM in DMSO and to 10 mM in ethanol with gentle warmingTocris Bioscience5075 |
| Soluble to 100 mM in DMSO and to 5 mM in ethanol with gentle warmingTocris Bioscience5075 |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 262-264 °CIndofine[H-005] |

* Miscellaneous

## Appearance:

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| --- |
| Off-White SolidIndofine[H-005] |

## Safety:

|  |
| --- |
| 20/22-36Alfa AesarL19068 |
| 26-36/37Alfa AesarL19068 |
| 9-26-36-60Alfa AesarL19068 |
| GHS08BiosynthH-1200 |
| H302-H332-H319Alfa AesarL19068 |
| H371BiosynthH-1200 |
| HARMFULAlfa AesarL19068 |
| P260; P309+P311BiosynthH-1200 |
| P280h-P305+P351+P338Alfa AesarL19068 |
| WarningAlfa AesarL19068 |
| WarningBiosynthH-1200 |

## Target Organs:

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| --- |
| MAO inhibitorsTargetMolT1711 |

## Chemical Class:

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| --- |
| alkaloidMicrosource[01500867] |

## Drug Status:

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| --- |
| experimentalMicrosource[01500867] |

## Compound Source:

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| Alkaloid from Peganum harmala, several Banisteriopsis spp., Passiflora edulis and several other spp. (Zygophyllaceae, Malphigiaceae, Passifloraceae)Zerenex Molecular[ZBioX-0190] |
| Peganium harmalaMicrosource[01500867] |

## Bio Activity:

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| --- |
| 5-HT ReceptorMedChem ExpressHY-N0737A |
| Antiparkinsonian agent; Zerenex Molecular[ZBioX-0190] |
| DYRKTocris Bioscience5075 |
| EnzymeTargetMolT1711 |
| EnzymesTocris Bioscience5075 |
| GPCR/G proteinMedChem ExpressHY-N0737A |
| GPCR/G protein; Neuronal Signaling; MedChem ExpressHY-N0737A |
| Harmine, a tricyclic b-carboline alkaloid that was originally; isolated from seeds of Peganum harmala, has been reported to possess anxiolytic, behavioral effects. MedChem ExpressHY-N0737A |
| KinasesTocris Bioscience5075 |
| MAOTargetMolT1711 |
| Potent and selective DYRK1A inhibitorTocris Bioscience5075 |
| Potent and selective inhibitor of DYRK1A (IC50 values are 80, 800 and 900 nM for DYRK1A, DYRK3 and DYRK2 respectively). Inhibits DYRK1A-mediated tau phosphorylation and regulates PPAR? expression. Also induces pancreatic beta cell proliferation. Exhibits antidiabetic activity. Orally bioavailable. Tocris Bioscience5075 |
| Potent and selective inhibitor of DYRK1A (IC50 values are 80, 800 and 900 nM for DYRK1A, DYRK3 and DYRK2 respectively). Shown to inhibit direct phosphorylation of tau by DYRK1A (IC50 = 700 nM). Also regulates PPAR? expression; exhibits antidiabetic activity. Orally bioavailable. Tocris Bioscience5075 |

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 1935 (estimated with error: 89)NIST Spectramainlib\_58654, replib\_116084, replib\_248286, replib\_379637 |

## Retention Index (Normal Alkane):

|  |
| --- |
| 2291 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Other; CAS no: 442513; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.)NIST Spectranist ri |

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

|  |  |
| --- | --- |
| Density: | 1. 3±0. 1 g/cm 3 |
| Boiling Point: | 421. 4±40. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±1. 0 mmHg at 25°C |
| Enthalpy of Vaporization: | 64. 9±3. 0 kJ/mol |
| Flash Point: | 139. 8±17. 0 °C |
| Index of Refraction: | 1. 706 |
| Molar Refractivity: | 66. 0±0. 3 cm 3 |
| #H bond acceptors: | 3 |
| #H bond donors: | 1 |
| #Freely Rotating Bonds: | 1 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 3. 17 |
| ACD/LogD (pH 5. 5): | 0. 49 |
| ACD/BCF (pH 5. 5): | 1. 00 |
| ACD/KOC (pH 5. 5): | 3. 46 |
| ACD/LogD (pH 7. 4): | 1. 61 |
| ACD/BCF (pH 7. 4): | 4. 78 |
| ACD/KOC (pH 7. 4): | 45. 40 |
| Polar Surface Area: | 38 Å 2 |
| Polarizability: | 26. 2±0. 5 10 -24 cm 3 |
| Surface Tension: | 55. 7±3. 0 dyne/cm |
| Molar Volume: | 169. 5±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) = 2. 83Log Kow (Exper. database match) = 3. 56Exper. Ref: Sangster (1994)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 380. 88 (Adapted Stein & Brown method)Melting Pt (deg C): 139. 17 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 4. 49E-008 (Modified Grain method)MP (exp database): 273 deg CSubcooled liquid VP: 2. 41E-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): 2. 676log Kow used: 3. 56 (expkow database)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 461. 84 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 39E-012 atm-m3/moleGroup Method: 6. 43E-010 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 686E-009 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 56 (exp database)Log Kaw used: -9. 520 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 13. 080Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8331Biowin2 (Non-Linear Model) : 0. 9438Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5971 (weeks-months)Biowin4 (Primary Survey Model) : 3. 5501 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3589Biowin6 (MITI Non-Linear Model): 0. 2056Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 0856Ready 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. 00321 Pa (2. 41E-005 mm Hg)Log Koa (Koawin est ): 13. 080Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 000934 Octanol/air (Koa) model: 2. 95 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0326 Mackay model : 0. 0695 Octanol/air (Koa) model: 0. 996 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 200. 9656 E-12 cm3/molecule-secHalf-Life = 0. 053 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 639 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 0511 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 329E+004Log Koc: 4. 124 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 = 2. 041 (BCF = 110)log Kow used: 3. 56 (expkow database)Volatilization from Water: Henry LC: 6. 43E-010 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 327E+006 hours (5. 527E+004 days)Half-Life from Model Lake : 1. 447E+007 hours (6. 03E+005 days)Removal In Wastewater Treatment: Total removal: 14. 47 percentTotal biodegradation: 0. 20 percentTotal sludge adsorption: 14. 27 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 0. 00969 1. 28 1000 Water 12. 6 900 1000 Soil 86. 3 1. 8e+003 1000 Sediment 1. 05 8. 1e+003 0 Persistence Time: 1. 64e+003 hr

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* 1-Click Scaffold Hop