Harmine c13h12n2o structure

Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_{13}H_{12}N_2O$
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:**

      338FooDBFDB0021

      49

- Experimental Physico-chemical Properties
    - **Experimental Melting Point:**

      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)LabNet

      workLN01307236

262-264

°CIndofine[H-005]

264-265 °C / 257

mmHgFooDBFDB0021

49

- **Experimental LogP:**

  3. 173Vitas-

  MSTK047386

- **Experimental Solubility:**

  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:**

    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:**

MAO

inhibitorsTargetMolT1711

- **Chemical Class:**

alkaloidMicrosource[0150

0867]

- **Drug Status:**

experimentalMicrosource[015

00867]

- **Compound Source:**

Alkaloid from

Peganum harmala, several Banisteriopsis spp., Passiflora edulis and several other spp. (Zygophyllaceae, Malphigiaceae, Passifloraceae)Zerenex Molecular[ZBioX-0190]

Peganum harmalaMicrosource[01500867]

- **Bio Activity:**

5-HT ReceptorMedChem ExpressHY-N0737A

Antiparkinsonian agent; Zerenex Molecular[ZBioX-0190]

DYRKTocris Bioscience5075

EnzymeTargetMolT17

11

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):**

    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