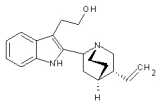

Formula: C19H24N2O

MW: 296.41

CAS: 482-28-0

TNP NUMBER: TNP00346

MDL NUMBER: MFCD06668150

IUPAC: 2-[2-((4S,8R)-8-vinylquinuclidin-2-yl)indol-3-yl]ethan-1-ol

Smiles: c1ccc2[nH]c(C3C[C@@H]4([C@H](C[N@@]3CC4)C=C))c(c2c1)CCO

ACCEPTORS: 1

DONORS: 2

ROTATION BONDS: 4

N+O: 3

Chiral Centers: 3

LogP: 4.48

LogS: -4.78

LIPINSKI: 4

Monograph Number: 0002306

Title: Cinchonamine

CAS Registry Number: 482-28-0

CAS Name: [1S-(1a,2a,4a,5b)]-2-(5-Ethenyl-1-azabicyclo[2.2.2]oct-2-yl)-1H-indole-3-ethanol

Additional Names: 3-(b-hydroxyethyl)-2-(5-vinyl-2-quinuclidyl)indole

Molecular Formula: C19H24N2O

Molecular Weight: 296.41.

Percent Composition: C 76.99%, H 8.16%, N 9.45%, O 5.40%

Literature References: From the bark of Remijia purdieana Wedd., Rubiaceae: Arnaud, Compt. Rend. 93, 593 (1881); Hesse, Ann. 225, 211 (1884). Prepn by reduction of quinamine with lithium aluminum hydride and structure: Goutarel et al., Helv. Chim. Acta 33, 150 (1950). Synthesis: Chen et al., C.A. 53, 7219e (1959). Total synthesis: G. Grethe et al., Helv. Chim. Acta 59, 2271 (1976). Stereochemistry: Wenkert, Bringi, J. Am. Chem. Soc. 80, 3484 (1958); Augustine, Chem. Ind. (London) 1959, 1071; Sawa, Matsumura, Tetrahedron 26, 2923 (1970). Biosynthetic studies: Battersby, Parry, Chem. Commun. 1971, 31. Conversion of chinchona alkaloids of the quinoline series to those of the indole series: Ochiai et al., C.A. 59, 14040h (1963).

Properties: Triboluminescent, orthorhombic prisms from methanol, mp 186, also reported as mp 194. [a]D20 +123 (c = 0.66 in ethanol). pK in 80% methyl Cellosolve: 8.28. uv max (methanol): 223, 292 nm (log e 4.60, 3.88). One gram dissolves in about 35 ml alcohol, 105 ml ether. Sol in benzene, chloroform, petr ether, CS2; practically insol in water.

Melting point: mp 186; mp 194

pKa: pK in 80% methyl Cellosolve: 8.28

Optical Rotation: [a]D20 +123 (c = 0.66 in ethanol)

Absorption maximum: uv max (methanol): 223, 292 nm (log e 4.60, 3.88)

Derivative Type: Hydrochloride monohydrate

Molecular Formula: C19H24N2O.HCl.H2O

Molecular Weight: 350.88.

Percent Composition: C 65.04%, H 7.76%, N 7.98%, O 9.12%, Cl 10.10%

Properties: Cubic crystals. One gram dissolves in 200 ml water. Sol in alc.

Synonyms:
cinchonamine;2-[(1S,4R)-(5B-Ethenyl-1-azabicyclo[2.2.2]oct-2a-yl)]-1H-indole-3-ethanol;2-[(1S,1a,4a)-5B-Ethenyl-1-azabicyclo[2.2.2]oct-2a-yl]-1H-indole-3-ethanol;2-[2-[(2S,4S,5R)-5-vinylquinuclidin-2-yl]-1H-indol-3-yl]ethanol;2-[2-[(4S,5R,7S)-5-ethenyl-1-azabicyclo[2.2.2]octan-7-yl]-1H-indol-3-yl]ethanol

CAS:482-28-0

MF:C19H24N2O

MW:0

EINECS:207-579-0

Product Categories: cinchonamine cinchonamine

Usage And Synthesis: cinchonamine