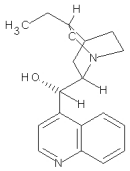

Formula: C19H24N2O

MW: 296.41

CAS: 485-65-4

MDL: MFCD00472868

TNP: TNP00118

LogP: 4.04

LogS: -5.02

Acceptors: 1

Donors: 1

Rotation Bonds: 3

Chiral Centers: 4

N+O: 3

LIPINSKY: 4

IUPAC: (1R)(5-ethylquinuclidin-2-yl)-4-quinolylmethan-1-ol

Smiles: c1(C(C2N3CC(CC)C(C2)CC3)O)c2c(ncc1)cccc2

Merck 13 Reference: Monograph Number: 0004804

Title: Hydrocinchonine

CAS Registry Number: 485-65-4

CAS Name: (9S)-10,11-Dihydrocinchonan-9-ol

Additional Names: cinchotine; cinconifine; (+)-dihydrocinchonine; pseudocinchonine

Molecular Formula: C19H24N2O

Molecular Weight: 296.41.

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

Literature References: From cinchona barks: Caventou, Willm, Compt. Rend. 69, 284 (1869). Prepn from cinchonine: Hesse, Ann. 300, 46 (1898); Pum, Monatsh. Chem. 16, 68 (1895); Arlt, ibid. 20, 426, 439 (1899); Heidelberger, Jacobs, J. Am. Chem. Soc. 41, 817 (1919). Structure: Rabe, Ber. 55, 522 (1922). Conversion of hydroquinidine to hydrocinchonine: King, J. Chem. Soc. 1946, 523. HPLC determn: C.-T. A. Chung, E. J. Staba, J. Chromatogr. 295, 276 (1984). Stereospecific synthesis from secologanin: R. T. Brown, D. Curless, Tetrahedron Lett. 27, 6005 (1986). Total synthesis: M. Ihara et al., J. Chem. Soc. Perkin Trans. 1 1988, 1277.

Properties: Prisms, mp 268-269. [a]D14 +204 (c = 0.6 in alc). Almost insol in water, ether. Sol in alcohol.

Melting point: mp 268-269

Optical Rotation: [a]D14 +204 (c = 0.6 in alc)

Derivative Type: Hydrochloride

Molecular Formula: C19H24N2O.HCl

Molecular Weight: 332.87.

Percent Composition: C 68.56%, H 7.57%, N 8.42%, O 4.81%, Cl 10.65%

Properties: Crystals, mp 220-221. [a]D23 +155 (c = 0.8 in water).

Melting point: mp 220-221

Optical Rotation: [a]D23 +155 (c = 0.8 in water)