



Formula: C₂₀H₂₄N₂O₂

MW: 324.42

CAS: 130-95-0

MDL: MFCD07808735

TNP: TNP00086



LogP: 2.89

LogS: -4.59

Acceptors: 2

Donors: 1

Rotation Bonds: 3

Chiral Centers: 4

N+O: 4

LIPINSKY: 4

IUPAC: (1R)((2S,4S,5R)-5-vinylquinuclidin-2-yl)(6-methoxy(4-quinolyl))methan-1-ol

Smiles: c1(C(C2N3CC(C=C)C(CC3)C2)O)c2c(ccc(c2)OC)ncc1

Merck 13 Reference: Percent Composition: C 74.04%, H 7.46%, N 8.63%, O 9.86%

Literature References: Primary alkaloid of various species of Cinchona (Rubiaceae), see Cinchona. Representative samples of dried bark contain ~0.8 to 4% quinine. Optical isomer of quinidine, q.v. Isoln: Pelletier, Caventau, Ann. Chem. Phys. [2], 15, 291 (1820). Extraction procedure: Jucker, Stoll, in Ullmanns Encyklop