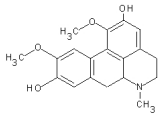

Formula: C19H21NO4

MW: 327.38

CAS: 476-70-0

MDL: MFCD00051180

TNP: TNP00245

(+)-(s)-boldine; (s)-boldine; (s)-yl; 1,10-dimethoxy-6a-alpha-aporphine-2,9-diol; 1,10-dimethoxy-6a-alpha-aporphine-9-diol; 4h-dibenzo(de,g)quinoline-2,9-diol,5,6,6a,7-tetrahydro-1,10-dimethoxy-6-meth; 4h-dibenzo[de,g]quinoline-2,9-diol,5,6,6a,7-tetrahydro-1,10

LogP: -4.73

LogS: -1.77

Acceptors: 4

Donors: 2

Rotation Bonds: 4

Chiral Centers: 1

N+O: 5

LIPINSKY: 4

Info: fro Boldo (Peumus Boldus)

IUPAC:

Smiles: c12c(cc(c(c1)OC)O)CC1N(CCc3c1c2c(c(c3)O)OC)C

Specification: Boldine Chemical Properties:

mp 162-164 C Merck 13,1316 CAS DataBase Reference476-70-0(CAS DataBase Reference) EPA Substance Registry System4H-Dibenzo[de,g] quinoline-2,9-diol, 5,6,6a,7-tetrahydro-1,10-dimethoxy- 6-methyl-, (6aS)-(476-70-0) Safety Information Hazard Codes Xn Risk Statements 22-36/37/38 Safety Statements 1-20-24/25-45-36-26 RIDADR 1544 WGK Germany 3 RTECS CE0750000 HazardClass 6.1(b) PackingGroup III Boldine Usage And Synthesis Boldine

Merck 13 Reference: Monograph Number: 0001316

Title: Boldine

CAS Registry Number: 476-70-0

CAS Name: 5,6,6a,7-Tetrahydro-1,10-dimethoxy-6-methyl-4H-dibenzo[de,g]quinoline-2,9-diol

Additional Names: 1,10-dimethoxy-6aa-aporphine-2,9-diol; 1,10-dimethoxy-2,9-dihydroxyaporphine; 2,6-dihydroxy-3,5-dimethoxyaporphine

Molecular Formula: C19H21NO4

Molecular Weight: 327.37.

Percent Composition: C 69.71%, H 6.47%, N 4.28%, O 19.55%

Literature References: Isoln from boldo (Peumus boldus Molina, Monimiaceae): Bourgoin, Verne, J. Pharm. Chim. 16, 191 (1872); from Laurelia novaezelandiae A. Cunn.: Bernauer, Helv. Chim. Acta 50, 1583 (1967). Structure: Warnat, Ber. 58, 2768; 59, 85 (1926); Sp