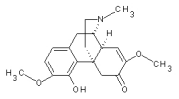

Formula: C19H23NO4

MW: 329.4

Salt: 0.3CHCl3

CAS: 115-53-7

MDL: MFCD01103301

TNP: TNP00111

7,8-didehydro-4-hydroxy-3,7-dimethoxy-17-methyl-9-alpha,13-alpha,14-alpha-mo; 9-alpha,13-alpha,14-alpha-morphinan-6-one,7,8-didehydro-4-hydroxy-3,7-dimethox; rphinan-6-one; y-17-methyl-; SABIANINE A; SINOMENIN; SINOMENINE; (9alpha,13alpha,14alpha)-7,8-didehydro-

LogP: 6.73

LogS: -5.43

Acceptors: 4

Donors: 1

Rotation Bonds: 3

Chiral Centers: 3

N+O: 5

LIPINSKY: 3

IUPAC: (9S,10S,1R)-3-hydroxy-4,12-dimethoxy-17-methyl-17-azatetracyclo[7.5.3.0.0]heptadeca-2,4,6,11-tetraen-13-one

Smiles: c12C34C(C=C(C(C3)=O)OC)C(Cc1ccc(c2O)OC)[N@](CC4)C

Specification: Alkaloids; Natural Plant Extract; Asymmetric Synthesis; Chiral Building Blocks; Complex Molecules Sinomenine Chemical Properties:

 mp 180 C (dec.)(lit.) storage temp. Store at +4C Merck 13,8620 Safety Information Hazard Codes T Risk Statements 45-46-23/24/25-36/37/38-20/21/22 Safety Statements 53-22-26-36/37/39-45 RIDADR 1544 WGK Germany 3 RTECS QD2170000 F 9 HazardClass 6.1(b) PackingGroup III (9alpha,13alpha,14alpha)-7,8-Didehydro-4-hydroxy-3,7-dimethoxy-17-methylmorphinan-6-one English Sinomenine Usage And Synthesis Biological ActivityNatural anti-inflammatory morphinan analog. Causes degranulation of mast cells in mammalian tissues to release histamine and suppresses production of proinflammatory cytokines. Also displays antinociceptive activity, possibly through activation of the