



Formula: C₂₉H₄₀N₂O₄

MW: 480.65

Salt: H₂O, 2HCl

CAS: 316-42-7

TNP NUMBER: TNP00093

MDL NUMBER: MFCD04220906

IUPAC: (1R)-1-(((10S,11aS,9R)-9-ethyl-2,3-dimethoxy(5,6,7,11a-tetrahydropiperidino[2,1-a]isoquinolin-10-yl))methyl)-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline, c hloride, hydrate

Smiles:

CCC1[C@@H](C[C@@H]2(c3cc(c(OC)cc3CCN2)OC))C[C@@H]2(N(C1)CCc1cc(OC)c(cc21)OC)

THERAPEUTIC CATEGORY: Antiamebic

REFERENCE: Meijerman I, et al., Induction of apoptosis and changes in nuclear G-actin are mediated by different pathways: the effect of inhibitors of protein and RNA synthesis in isolated rat hepatocytes. *Toxicol. Appl. Pharmacol.* 156(1), 46-55, (1999) Hikawa, N., and Takenaka, T., Method for production of neuronal hybridoma using emetine and actinomycin D. *Brain Res. Brain Res. Protoc.* 1, 224-226, (1997) Galasinski W., et al., The substances of plant origin that inhibit protein biosynthesis. *Acta Pol. Pharm.* 53, 311-318, (1996) abstract Merck Merck 13,3591 Beilstein Beil. 23,IV,3419

SOURCE: Principal alkaloid of ipecac, the ground roots of *Uragoga ipecacuaha* (Brot.) Baill. Rubiaceae; occurs naturally as (-)-form

ACCEPTORS: 4

DONORS: 1

ROTATION BONDS: 6

N+O: 6

Chiral Centers: 4

LogP: 6.13

LogS: -6.08

LIPINSKI: 3

Synonyms: (+)-EMETINE DIHYDROCHLORIDE HYDRATE;EMETINE DIHYDROCHLORIDE HYDRATE

CAS:

MF:C29H44Cl2N2O5

MW:571.58

EINECS:206-259-8

Product Categories: (+)-EMETINE DIHYDROCHLORIDE HYDRATE

Chemical Properties: mp 240-250 C (dec., dry matter)(lit.) storage temp. 2-8C T+ Risk Statements 28-36/37/38 Safety Statements 26-28-36/37-45 RIDADR UN 1544 6.1/PG 2 WGK Germany 3 RTECS JY5250000 F 3-8-10 (+)-EMETINE DIHYDROCHLORIDE HYDRATE

Usage And Synthesis: (+)-EMETINE DIHYDROCHLORIDE HYDRATE

