Emetine

Other names: Emetan, 6',7',10,11-tetramethoxy-
2H-Benzo(a)quinolizine, 3-ethyl-1,3,4,6,7,11b-hexahydro-9,10-dimethoxy-2-((1,2,3,4-tetrahydro-6,7-dimethoxy-1-is
Cephaeline methyl ether
NSC 33669
6',7',10,11-Tetramethoxyemetan
Emetin
316-42-7 (chloride)

Inchi: InChI=1S/C29H40N2O4/c1-6-18-17-31-10-8-20-14-27(33-3)29(35-5)16-23(20)25(31)12-2

InchiKey: AUVVAXYIELKVAI-UHFFFAOYSA-N

Formula: C29H40N2O4

SMILES: CCC1CN2CCc3cc(OC)c(OC)cc3C2CC1CC1NCCc2cc(OC)c(OC)cc21

Mol. weight [g/mol]: 480.64

CAS: 483-18-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	4.943		Crippen Method
mcvol	382.810	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C483181&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume