

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- 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
mcpol	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

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