Aconitine

Other names:	Aconitane-3,8,13,14,15-pentol, 20-ethyl-1,6,16-trimethoxy-4-(methoxymethyl)-, 8-acetate 14-benzoate, (1«alpha»,3«alpha»,6«alpha»,14«alpha»,15«alpha»,16«beta»)- Aconitane Aconitin cristallisat 2H-12,3,6a-Ethanylylidene-7,9-methanonaphth[2,3-b]azocine, aconitane-3,8,13,14,15-pentol deriv.
Inchi:	InChI=1S/C34H47NO11/c1-7-35-15-31(16-41-3)20(37)13-21(42-4)33-19-14-32(40)28(45
InchiKey:	XFSBVAOIAHNAPC-UHFFFAOYSA-N
Formula:	C34H47NO11
SMILES:	CCN1CC2(COC)C(O)CC(OC)C34C5CC6(O)C(OC)C(O)C(OC(C)=O)(C5C6OC(=O)c5cc
Mol. weight [g/mol]:	645.74
CAS:	302-27-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	0.648		Crippen Method
mcvol	466.950	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C302272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from: