O-Acetylcrotavernine

Inchi: InChI=1S/C21H29NO7/c1-6-15-11-13(2)21(4,29-14(3)23)20(26)27-12-16-7-9-22(5)10-8-1
InchiKey: ZOIAVVNLMDKOIV-BPYQQJMWSA-N
Formula: C21H29NO7
SMILES: CC=C1CC(C)C(C)(OC(C)=O)C(=O)OCC2=CCN(C)CCC(OC1=O)C2=O
Mol. weight [g/mol]: 407.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	1.580		Crippen Method
mcvol	310.300	ml/mol	McGowan Method
rinpol	2830.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R590311&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices