

Floridanine (otonecine-acetyljacoline)

Inchi: InChI=1S/C21H31NO9/c1-12-10-21(28,13(2)23)19(27)30-16-7-9-22(5)8-6-15(17(16)25)1
InchiKey: MPJBVZKNLCGQHF-XAHVSKGQSA-N
Formula: C21H31NO9
SMILES: CC(=O)OC1(C)C(=O)OCC2=CCN(C)CCC(OC(=O)C(O)(C(C)O)CC1C)C2=O
Mol. weight [g/mol]: 441.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	-0.254		Crippen Method
mcvol	326.340	ml/mol	McGowan Method
rinpol	2755.00		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2755.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R178184&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

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<https://www.chemeo.com/cid/55-371-9/Floridanine-otonecine-acetyljacoline.pdf>

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