Floricaline (otonecine-diacetyljacoline)

Inchi: InChI=1S/C23H33NO10/c1-13-11-23(30,14(2)32-15(3)25)21(29)33-18-8-10-24(6)9-7-17(
InchiKey: IVVHMCWHYZBIAK-QHAHYZBVSA-N
Formula: C23H33NO10
SMILES: CC(=O)OC(C)C1(O)CC(C)C(C)(OC(C)=O)C(=O)OCC2=CCN(C)CCC(OC1=O)C2=O
Mol. weight [g/mol]: 483.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.86		Crippen Method
logp	0.317		Crippen Method
mcvol	356.090	ml/mol	McGowan Method
rinpol	2846.00		NIST Webbook
rinpol	2852.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R178179&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
rinpol: Non-polar retention indices

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