Florosenine (otonecine-acetyljacobine)

Inchi: InChI=1S/C21H29NO8/c1-12-10-21(13(2)29-21)19(26)28-16-7-9-22(5)8-6-15(17(16)24)1
InchiKey: RNNVXCSFOWGBQP-BTKMTZEGSA-N
Formula: C21H29NO8
SMILES: CC(=O)OC1(C)C(=O)OCC2=CCN(C)CCC(OC(=O)C3(CC1C)OC3C)C2=O
Mol. weight [g/mol]: 423.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	0.792		Crippen Method
mcvol	309.610	ml/mol	McGowan Method
rinpol	2745.00		NIST Webbook
rinpol	2750.00		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=R177894&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.