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:	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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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