Doronine (otonecine-acetyljaconine)

Inchi: InChI=1S/C21H30ClNO8/c1-12-10-21(28,13(2)22)19(27)30-16-7-9-23(5)8-6-15(17(16)25
InchiKey: VGRSISYREBBIAL-HOVRZMKWSA-N
Formula: C21H30ClNO8
SMILES: CC(=O)OC1(C)C(=O)OCC2=CCN(C)CCC(OC(=O)C(O)(C(C)Cl)CC1C)C2=O
Mol. weight [g/mol]: 459.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Crippen Method
logp	0.992		Crippen Method
mcvol	332.710	ml/mol	McGowan Method
rinpol	2780.00		NIST Webbook
rinpol	2789.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R178159&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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