Desacetyldoronine (otonecin-jaconine)

Inchi: InChI=1S/C19H28ClNO7/c1-11-9-19(26,12(2)20)17(24)28-14-6-8-21(4)7-5-13(15(14)22)
InchiKey: OMHSMPLRLNEBIB-KLVGJWEWSA-N
Formula: C19H28ClNO7
SMILES: CC1CC(O)(C(C)Cl)C(=O)OC2CCN(C)CC=C(COC(=O)C1(C)O)C2=O
Mol. weight [g/mol]: 417.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	0.422		Crippen Method
mcvol	302.960	ml/mol	McGowan Method
rinpol	2660.00		NIST Webbook
rinpol	2676.00		NIST Webbook
rinpol	2660.00		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=R178144&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