

Otosenine

Inchi: InChI=1S/C19H27NO7/c1-11-9-19(12(2)27-19)17(23)26-14-6-8-20(4)7-5-13(15(14)21)10
InchiKey: CZQLULNMKQAIQL-KZNVHYRYSA-N
Formula: C19H27NO7
SMILES: CC1CC2(OC2C)C(=O)OC2CCN(C)CC=C(COC(=O)C1(C)O)C2=O
Mol. weight [g/mol]: 381.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.45		Crippen Method
logp	0.221		Crippen Method
mcvol	279.860	ml/mol	McGowan Method
rinpol	2631.00		NIST Webbook
rinpol	2595.00		NIST Webbook
rinpol	2601.00		NIST Webbook
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
rinpol	2595.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R177923&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

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