Axillarine

Inchi: InChI=1S/C18H27NO7/c1-9(2)13-15(21)18(24,10(3)20)17(23)25-8-11-4-6-19-7-5-12(14(1
InchiKey: JGQRXNDIMGIXDT-CYWQAWCWSA-N
Formula: C18H27NO7
SMILES: CC(C)C1C(=O)OC2CCN3CC=C(COC(=O)C(O)(C(C)O)C1O)C23
Mol. weight [g/mol]: 369.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	-0.786		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
rinpol	2563.00		NIST Webbook
rinpol	2569.00		NIST Webbook
rinpol	2563.00		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=R178124&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