Desoxyaxillarine

Inchi:	InChI=1S/C18H27NO6/c1-10(2)13-8-18(23,11(3)20)17(22)24-9-12-4-6-19-7-5-14(15(12)1
InchiKey:	QFUAXLZCUKBODH-GKHXFJEZSA-N
Formula:	C18H27NO6
SMILES:	CC(C)C1CC(O)(C(C)O)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]:	353.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	0.244		Crippen Method
mcvol	264.200	ml/mol	McGowan Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R178411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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