3'-acetylsupinine

Inchi:	InChI=1S/C17H27NO6/c1-10(2)17(22,11(3)24-12(4)19)16(21)23-9-13-5-7-18-8-6-14(20)
InchiKey:	YFQPDKABPCMKCA-PEQUQEEVSA-N
Formula:	C17H27NO6
SMILES:	CC(=O)OC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)C
Mol. weight [g/mol]:	341.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	0.244		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		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=R240487&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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