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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.