7-diacetyllycopsamine

Inchi: InChI=1S/C19H29NO7/c1-11(2)19(24,12(3)26-13(4)21)18(23)25-10-15-6-8-20-9-7-16(17
InchiKey: JBYCUUBCNYWXMY-FYENTVDSSA-N
Formula: C19H29NO7
SMILES: CC(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)C)C(C)OC(C)=O)C12
Mol. weight [g/mol]: 383.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	0.814		Crippen Method
mcvol	290.720	ml/mol	McGowan Method
rinpol	2340.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R227895&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