

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:	JBYCUUBCNVWXYMY-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

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<https://www.chemeo.com/cid/30-298-8/7-diacetyllycopsamine.pdf>

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