13-Propionyloxy-lupanine

Other names: 13-propyloxylupanine
Inchi: InChI=1S/C18H28N2O3/c1-2-18(22)23-15-5-7-19-13(10-15)8-12-9-14(19)11-16-17(21)4-
InchiKey: OEQFCMUGHQTLOJ-UHFFFAOYSA-N
Formula: C18H28N2O3
SMILES: CCC(=O)OC1CCN2C(C1)CC1CC2CC2C(=O)CCCN12
Mol. weight [g/mol]: 320.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	1.741		Crippen Method
mcvol	250.010	ml/mol	McGowan Method
rinpol	2555.00		NIST Webbook
rinpol	2530.00		NIST Webbook
rinpol	2555.00		NIST Webbook
rinpol	2530.00		NIST Webbook

Sources

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=R261271&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices