

13-isovaleroyloxylupanine

Inchi: InChI=1S/C20H32N2O3/c1-13(2)8-20(24)25-16-6-7-21-11-14-9-15(18(21)10-16)12-22-17
InchiKey: VFLZLHQEIKPJJCQ-AFKOE00ISA-N
Formula: C20H32N2O3
SMILES: CC(C)CC(=O)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.439		Crippen Method
mcvol	278.190	ml/mol	McGowan Method
rinpol	2685.00		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=R390275&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

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<https://www.chemeo.com/cid/39-794-8/13-isovaleroyloxylupanine.pdf>

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