13«alpha»-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: VFLZLHQEIKPJCQ-HNICDYJYSA-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	2714.00		NIST Webbook
rinpol	2680.00		NIST Webbook
rinpol	2714.00		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=R205375&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