13-(2-Methylbutyryl)oxylupanine

Inchi: InChI=1S/C20H32N2O3/c1-3-13(2)20(24)25-16-7-8-21-11-14-9-15(18(21)10-16)12-22-17

InchiKey: KMPISACSSNDWOU-XTWABXLZSA-N

Formula: C20H32N2O3

SMILES: CCC(C)C(=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	2655.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R598548&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