13-Isobutyryloxylupanine

Inchi: InChI=1S/C19H30N2O3/c1-12(2)19(23)24-15-6-7-20-10-13-8-14(17(20)9-15)11-21-16(13
InchiKey: FOPGUSZPKIVDDA-WALXCBACSA-N
Formula: C19H30N2O3
SMILES: CC(C)C(=O)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	2.049		Crippen Method
mcvol	264.100	ml/mol	McGowan Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R598593&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.