13«alpha»-Butyryloxylupanine

Inchi: InChI=1S/C19H30N2O3/c1-2-4-19(23)24-15-7-8-20-11-13-9-14(17(20)10-15)12-21-16(13
InchiKey: QZEIXRNLIXRJMJ-AYXGTZKJSA-N
Formula: C19H30N2O3
SMILES: CCCC(=O)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.193		Crippen Method
mcvol	264.100	ml/mol	McGowan Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2620.00		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=R205360&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