13«alpha»-Propyonyloxylupanine

Inchi: InChI=1S/C18H28N2O3/c1-2-18(22)23-14-6-7-19-10-12-8-13(16(19)9-14)11-20-15(12)4-
InchiKey: CCMRUNUIUBUKPX-GMOYYMRRSA-N
Formula: C18H28N2O3
SMILES: CCC(=O)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 320.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.803		Crippen Method
mcvol	250.010	ml/mol	McGowan Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		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=R557027&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

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