13«alpha»-Acetyloxylupanine

Inchi: InChI=1S/C17H26N2O3/c1-11(20)22-14-5-6-15-13-7-12(8-18(15)10-14)16-3-2-4-17(21)1
InchiKey: YNKXIAFLUMVBNM-GMOYYMRRSA-N
Formula: C17H26N2O3
SMILES: CC(=O)OC1CCC2C3CC(CN2C1)C1CCCC(=O)N1C3
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	1.413		Crippen Method
mcvol	235.920	ml/mol	McGowan Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook

Sources

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=R263806&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices