13«beta»-hydroxylupanine

Inchi: InChI=1S/C15H24N2O2/c18-12-4-5-16-8-10-6-11(14(16)7-12)9-17-13(10)2-1-3-15(17)19
InchiKey: JVYKIBAJVKEZSQ-DMTXQYTPSA-N
Formula: C15H24N2O2
SMILES: O=C1CCCC2C3CC(CN12)C1CC(O)CCN1C3
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	0.842		Crippen Method
mcvol	206.170	ml/mol	McGowan Method
rinpol	2405.00		NIST Webbook
rinpol	2405.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R322108&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.