

15«beta»-Hydroxy-17-oxolupanine

Inchi: InChI=1S/C15H22N2O3/c18-13-5-2-4-12-10-7-9(8-16(12)13)11-3-1-6-14(19)17(11)15(10)
InchiKey: DUWSBJYHDRCLCG-KCCZXEEPSA-N
Formula: C15H22N2O3
SMILES: O=C1CCCC2C3CC(CN12)C1CCCC(O)N1C3=O
Mol. weight [g/mol]: 278.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.98		Crippen Method
logp	0.717		Crippen Method
mcvol	207.740	ml/mol	McGowan Method
rinpola	2646.00		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=R557067&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
rinpola: Non-polar retention indices

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