

oxolupanine

Inchi: InChI=1S/C15H20N2O2/c18-14-6-3-5-12-10-8-11(15(19)17(12)14)13-4-1-2-7-16(13)9-10
InchiKey: HDEXKFWRBAIRHI-UHFFFAOYSA-N
Formula: C15H20N2O2
SMILES: O=C1CCC=C2C3CC(C(=O)N12)C1CCCCN1C3
Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	1.523		Crippen Method
mcvol	197.570	ml/mol	McGowan Method
rinpola	2345.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R320682&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
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/59-309-4/oxolupanine.pdf>

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