Hydroxyaphyllidine

Inchi: InChI=1S/C15H22N2O2/c18-14-6-3-5-12-10-8-11(15(19)17(12)14)13-4-1-2-7-16(13)9-10
InchiKey: JHXYFYGGFKMUPN-UHFFFAOYSA-N
Formula: C15H22N2O2
SMILES: O=C1C2CC(CN3CCCCC23)C2=CCCC(O)N12
Mol. weight [g/mol]: 262.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	1.315		Crippen Method
mcvol	201.870	ml/mol	McGowan Method
rinpol	2217.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R281037&Units=SI
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

Legend

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