

1-[[[(1S)-2,3,4,6,7,8,9,9a-Octahydro-1H-quinolizin-1-

Inchi:	InChI=1S/C14H22N2O2/c17-13-6-7-14(18)16(13)10-11-4-3-9-15-8-2-1-5-12(11)15/h11-1
InchiKey:	AWFORQRBTPBAMY-PXYINDEMSA-N
Formula:	C14H22N2O2
SMILES:	O=C1CCC(=O)N1CC1CCCN2CCCCC12
Mol. weight [g/mol]:	250.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	1.400		Crippen Method
mcvol	198.640	ml/mol	McGowan Method
rinpole	2060.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R577665&Units=SI

Legend

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

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