Dehydrocytisine

Inchi: InChI=1S/C11H12N2O/c14-11-3-1-2-10-9-4-8(5-12-6-9)7-13(10)11/h1-3,6,8-9H,4-5,7H2
InchiKey: CSPJATRBHWXIFP-UHFFFAOYSA-N
Formula: C11H12N2O
SMILES: O=c1cccc2n1CC1CN=CC2C1
Mol. weight [g/mol]: 188.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	1.036		Crippen Method
mcvol	141.900	ml/mol	McGowan Method
rinpol	1972.00		NIST Webbook
rinpol	1977.00		NIST Webbook
rinpol	1977.00		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=R264141&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
rinpol: Non-polar retention indices