

Dehydro-sparteine

Inchi: InChI=1S/C15H24N2/c1-3-7-16-11-13-9-12(14(16)5-1)10-17-8-4-2-6-15(13)17/h3,7,12-14
InchiKey: BWKNRAAXVUYXAH-ZQDZILKHS-A-N
Formula: C15H24N2
SMILES: C1=CN2CC3CC(CN4CCCCC34)C2CC1
Mol. weight [g/mol]: 232.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.469		Crippen Method
mcvol	194.430	ml/mol	McGowan Method
rinpol	1810.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1840.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109178&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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
rinpol: Non-polar retention indices

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