11,12-Dehydrosparteine

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/h1,5,12-15
InchiKey:	CEGRSKIFIBSIQU-PFSRBDOWSA-N
Formula:	C15H24N2
SMILES:	C1=CC2C3CC(CN2CC1)C1CCCCN1C3
Mol. weight [g/mol]:	232.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	2.121		Crippen Method
mcvol	194.430	ml/mol	McGowan Method
rinpol	1840.00		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=R598528&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

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