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-UHFFFAOYSA-N

Formula: C15H24N2

SMILES: C1=CC2C3CC(CN2CC1)C1CCCCN1C3

Mol. weight [g/mol]: 232.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Cheméo Relay (1.0)
logp	2.121		Crippen Method
mcvol	194.430	ml/mol	McGowan Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1833.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R261231&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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