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]: 232.37

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

Sources

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

Cheméo Relay (1.0):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume