

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/h1,5,12-14
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

Latest version available from:

<https://www.chemeo.com/cid/83-632-8/11-12-dehydrosparteine.pdf>

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