11,12-Dehydrosparteine isomer

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/h5,12-13,1

InchiKey: YIHBNZCJQJSZJP-UHFFFAOYSA-N

Formula: C15H24N2

SMILES: C1=C2C3CC(CN2CCC1)C1CCCCN1C3

Mol. weight [g/mol]: 232.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	2.470		Crippen Method
mcvol	194.430	ml/mol	McGowan Method
rinpol	1822.00		NIST Webbook

Sources

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

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=R588957&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices