14-hydroxysparteine

Other names: hydroxysparteine
Inchi: InChI=1S/C15H26N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h11
InchiKey: AFEKUFYCNWZEGZ-UHFFFAOYSA-N
Formula: C15H26N2O
SMILES: OC1CCCC2C3CC(CN12)C1CCCCN1C3
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.78		Cheméo Relay (1.0)
logp	1.664		Crippen Method
mcvol	204.600	ml/mol	McGowan Method
rinpol	2055.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2052.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2055.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R261320&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):
Cheméo Relay (1.0, beta):

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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