

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	-2.43		Crippen Method
logp	1.664		Crippen Method
mcvol	204.600	ml/mol	McGowan Method
rinpol	2055.00		NIST Webbook
rinpol	2052.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2052.00		NIST Webbook
rinpol	2050.00		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=R261320&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

Latest version available from:

<https://www.chemeo.com/cid/83-650-8/14-hydroxysparteine.pdf>

Generated by Cheméo on 2024-04-28 08:51:51.778618249 +0000 UTC m=+16583560.699195565.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.