

17-Oxo-«beta»-isosparteine

Inchi: InChI=1S/C15H24N2O/c18-15-11-9-17-8-4-2-6-14(17)12(15)10-16-7-3-1-5-13(11)16/h11
InchiKey: GHGQXOFLRGUXQS-UHFFFAOYSA-N
Formula: C15H24N2O
SMILES: O=C1C2CN3CCCCC3C1CN1CCCCC21
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.84		Crippen Method
logp	1.524		Crippen Method
mcvol	200.300	ml/mol	McGowan Method
rinpol	2182.00		NIST Webbook
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Sources

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=R264007&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/93-409-5/17-Oxo-beta-isosparteine.pdf>

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