

7-Hydroxy-«beta»-isosparteine

Inchi: InChI=1S/C15H26N2O/c18-15-9-12(10-16-7-4-2-6-14(15)16)13-5-1-3-8-17(13)11-15/h12
InchiKey: DUUGVIKWQIWALC-URGYJCLVSA-N
Formula: C15H26N2O
SMILES: OC12CC(CN3CCCCC31)C1CCCCN1C2
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	1.460		Crippen Method
mcvol	204.600	ml/mol	McGowan Method
rinpol	1965.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1965.00		NIST Webbook

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=R577927&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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