

dehydro-oxosparteine

Inchi: InChI=1S/C15H22N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h3,6-14,17-18,21-22
InchiKey: YDYCLZUDFBNNQE-WCFLAILDSA-N
Formula: C15H22N2O
SMILES: O=C1C=CCC2C3CC(CN12)C1CCCCN1C3
Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	1.648		Crippen Method
mcvol	196.000	ml/mol	McGowan Method
rinpola	2120.00		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=R398393&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvola: McGowan's characteristic volume
rinpola: Non-polar retention indices

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