

Spartioidine

Inchi: InChI=1S/C18H23NO5/c1-4-12-9-11(2)18(3,22)17(21)23-10-13-5-7-19-8-6-14(15(13)19)
InchiKey: FCEVNJIUIMLVML-PBQSOSRTSA-N
Formula: C18H23NO5
SMILES: C=C1CC(=CC)C(=O)OC2CCN3CC=C(COC(=O)C1(C)O)C23
Mol. weight [g/mol]: 333.38
CAS: 520-59-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	1.113		Crippen Method
mcvol	249.730	ml/mol	McGowan Method
rinpol	2400.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2345.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C520592&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/43-137-2/Spartioidine.pdf>

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