

# 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	2359.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2359.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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>  
**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

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