

# Riddelliine

**Inchi:** InChI=1S/C18H23NO6/c1-3-12-8-11(2)18(23,10-20)17(22)24-9-13-4-6-19-7-5-14(15(13))  
**InchiKey:** SVCNNZDUGWLODJ-QJOXTKROSA-N  
**Formula:** C18H23NO6  
**SMILES:** C=C1CC(=CC)C(=O)OC2CCN3CC=C(COC(=O)C1(O)CO)C23  
**Mol. weight [g/mol]:** 349.38  
**CAS:** 23246-96-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	0.085		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23246960&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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