

# Isocreatonotine

**Inchi:** InChI=1S/C13H21NO4/c1-8(2)12(16)13(17)18-10-4-6-14-5-3-9(7-15)11(10)14/h3,8,10-12  
**InchiKey:** YVFZQQHFBSOTJ-PRWSFJOGSA-N  
**Formula:** C13H21NO4  
**SMILES:** CC(C)C(O)C(=O)OC1CCN2CC=C(CO)C12  
**Mol. weight [g/mol]:** 255.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.96		Crippen Method
logp	-0.078		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
rinpola	1960.00		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=R178446&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  
**rinpola:** Non-polar retention indices

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