

# 5-(2-Oxopropyl)hygrine

**Inchi:** InChI=1S/C11H19NO2/c1-8(13)6-10-4-5-11(12(10)3)7-9(2)14/h10-11H,4-7H2,1-3H3  
**InchiKey:** JIAAQKAOFZRDCM-UHFFFAOYSA-N  
**Formula:** C11H19NO2  
**SMILES:** CC(=O)CC1CCC(CC(C)=O)N1C  
**Mol. weight [g/mol]:** 197.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	1.407		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
rinpol	1442.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R509885&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

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