

# 21-Hydroxyintergerrimine

**Inchi:** InChI=1S/C18H25NO6/c1-11-9-12(5-8-20)16(21)25-14-4-7-19-6-3-13(15(14)19)10-24-17  
**InchiKey:** NSKVSAYYBLAAGQ-ARKXZKMKSA-N  
**Formula:** C18H25NO6  
**SMILES:** CC1CC(=CCO)C(=O)OC2CCN3CC=C(COC(=O)C1(C)O)C23  
**Mol. weight [g/mol]:** 351.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	0.165		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R636472&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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