

# Histamine, iso-BOC

**Inchi:** InChI=1S/C15H25N3O4/c1-11(2)8-21-14(19)16-6-5-13-7-18(10-17-13)15(20)22-9-12(3)4  
**InchiKey:** AUGRFJQUKDWQCT-UHFFFAOYSA-N  
**Formula:** C15H25N3O4  
**SMILES:** CC(C)COC(=O)NCCc1cn(C(=O)OCC(C)C)cn1  
**Mol. weight [g/mol]:** 311.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	2.449		Crippen Method
mcvol	247.570	ml/mol	McGowan Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		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=R392479&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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