

# Histapyrrodine M (N-desbenzyl-oxo), acetylated

**Inchi:** InChI=1S/C14H18N2O2/c1-12(17)16(13-7-3-2-4-8-13)11-14(18)15-9-5-6-10-15/h2-4,7-8  
**InchiKey:** ANADNQXPDLZISJ-UHFFFAOYSA-N  
**Formula:** C14H18N2O2  
**SMILES:** CC(=O)N(CC(=O)N1CCCC1)c1ccccc1  
**Mol. weight [g/mol]:** 246.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	1.662		Crippen Method
mcvol	196.600	ml/mol	McGowan Method
rinpola	2160.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R536431&Units=SI>  
**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)

## 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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