

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

**Inchi:** InChI=1S/C15H20N2O2/c1-13(18)17(11-14-7-3-2-4-8-14)12-15(19)16-9-5-6-10-16/h2-4,7-10,12-14,16-18,20-21  
**InchiKey:** WCBMPKHDDLDEO-UHFFFAOYSA-N  
**Formula:** C15H20N2O2  
**SMILES:** CC(=O)N(CC(=O)N1CCCC1)Cc1ccccc1  
**Mol. weight [g/mol]:** 260.33

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.28   |        | Crippen Method |
| logp          | 1.658   |        | Crippen Method |
| mcvol         | 210.690 | ml/mol | McGowan Method |
| rinpola       | 2260.00 |        | NIST Webbook   |
| rinpola       | 2260.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R536451&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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