# Histamine, N,N',N'-triacetyl-

**Inchi:** InChI=1S/C11H15N3O3/c1-8(15)13-6-11(12-7-13)4-5-14(9(2)16)10(3)17/h6-7H,4-5H2,1-
**InchiKey:** NDNZBWUEKDZBEN-UHFFFAOYSA-N
**Formula:** C11H15N3O3
**SMILES:** CC(=O)N(CCc1cn(C(C)=O)cn1)C(C)=O
**Mol. weight [g/mol]:** 237.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.95 | | Crippen Method |
| logp | 0.481 | | Crippen Method |
| mcvol | 181.040 | ml/mol | McGowan Method |
| rinpol | 1963.00 | | NIST Webbook |
| rinpol | 1963.00 | | NIST Webbook |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U374885&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** 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
**rinpol:** Non-polar retention indices

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