

# Hydrouracil, 1-nitroso-

**Inchi:** InChI=1S/C4H5N3O3/c8-3-1-2-7(6-10)4(9)5-3/h1-2H2,(H,5,8,9)  
**InchiKey:** NTUQAPWIPWIIWLT-UHFFFAOYSA-N  
**Formula:** C4H5N3O3  
**SMILES:** O=NN1CCC(=O)NC1=O  
**Mol. weight [g/mol]:** 143.10  
**CAS:** 16813-36-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	-0.390		Crippen Method
mcvol	91.010	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16813368&Units=SI>  
**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>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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