

# 3-Acetamido-5-acetylfuran

**Inchi:** InChI=1S/C8H9NO3/c1-5(10)8-3-7(4-12-8)9-6(2)11/h3-4H,1-2H3,(H,9,11)  
**InchiKey:** GPLHPEIJJXDRBA-UHFFFAOYSA-N  
**Formula:** C8H9NO3  
**SMILES:** CC(=O)Nc1coc(C(C)=O)c1  
**Mol. weight [g/mol]:** 167.16  
**CAS:** 95598-28-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	1.441		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C95598280&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  
**rinpol:** Non-polar retention indices

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