

# Pyrimidine, 6-oxo-5-acetyl-4-hydroxy-1,6-dihydro-

Other names:	6-Hydroxy-5-acetyl-4-oxo-1,6-dihydropyrimidine
Inchi:	InChI=1S/C6H6N2O3/c1-3(9)4-5(10)7-2-8-6(4)11/h2H,1H3,(H2,7,8,10,11)
InchiKey:	PYJZBCIQPVBBPY-UHFFFAOYSA-N
Formula:	C6H6N2O3
SMILES:	CC(=O)c1c(O)nc[nH]c1=O
Mol. weight [g/mol]:	154.12
CAS:	98792-81-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.09		Crippen Method
logp	-0.804		Crippen Method
mcvol	104.910	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C98792815&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C98792815&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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