

# 3-Acetyl-1H-pyrroline

<b>Other names:</b>	3-Acetylpyrrole
<b>Inchi:</b>	InChI=1S/C6H7NO/c1-5(8)6-2-3-7-4-6/h2-4,7H,1H3
<b>InchiKey:</b>	KHHSXHXUQVNBGA-UHFFFAOYSA-N
<b>Formula:</b>	C6H7NO
<b>SMILES:</b>	CC(=O)c1cc[nH]c1
<b>Mol. weight [g/mol]:</b>	109.13
<b>CAS:</b>	1072-82-8

## Physical Properties

Property code	Value	Unit	Source
hsub	94.70 ± 0.50	kJ/mol	NIST Webbook
log10ws	-1.35		Crippen Method
logp	0.735		Crippen Method
mcvol	87.490	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	93.20 ± 0.50	kJ/mol	327.00	NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072828&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072828&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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