

# 1H-Imidazole, 1-acetyl-

<b>Other names:</b>	Imidazole, 1-acetyl- Acetylimidazole N-Acetylimidazole 1-Acetylimidazole Imidazole, N-acetyl- 1-Acetyl-1H-imidazole
<b>Inchi:</b>	InChI=1S/C5H6N2O/c1-5(8)7-3-2-6-4-7/h2-4H,1H3
<b>InchiKey:</b>	VIHYIVKKEECZGOU-UHFFFAOYSA-N
<b>Formula:</b>	C5H6N2O
<b>SMILES:</b>	CC(=O)n1ccnc1
<b>Mol. weight [g/mol]:</b>	110.11
<b>CAS:</b>	2466-76-4

## Physical Properties

Property code	Value	Unit	Source
ie	9.38	eV	NIST Webbook
log10ws	-1.36		Crippen Method
logp	0.543		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
rinpola	1054.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2466764&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2466764&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

**ie:** Ionization energy

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcpol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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