

# 5-acetyl-2,3-1H-pyrrolizine

<b>Other names:</b>	5-acetyl-2,3-dihydro-1H-pyrrolizine 5-acetyl-2,3-dihydro-1H-pyrrolizine
<b>Inchi:</b>	InChI=1S/C9H11NO/c1-7(11)9-5-4-8-3-2-6-10(8)9/h4-5H,2-3,6H2,1H3
<b>InchiKey:</b>	NWSCEJHRUVCUSX-UHFFFAOYSA-N
<b>Formula:</b>	C9H11NO
<b>SMILES:</b>	CC(=O)c1ccc2n1CCC2
<b>Mol. weight [g/mol]:</b>	149.19
<b>CAS:</b>	55041-85-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	1.637		Crippen Method
mccvol	118.900	ml/mol	McGowan Method
rinpol	1335.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1354.00		NIST Webbook
ripol	2033.00		NIST Webbook
ripol	2021.00		NIST Webbook
ripol	2021.00		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=C55041855&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55041855&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

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices  
**ripol:** Polar retention indices

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