

# Ethanone, 1-(2,4-dimethyl-1H-pyrrol-3-yl)-

<b>Other names:</b>	Ketone, 2,4-dimethylpyrrol-3-yl methyl 2,4-Dimethyl-3-acetylpyrrole 2,4-Dimethylpyrrol-3-yl methyl ketone 3-Acetyl-2,4-dimethylpyrrole 1-(2,4-Dimethyl-1H-pyrrol-3-yl)-ethanone
<b>Inchi:</b>	InChI=1S/C8H11NO/c1-5-4-9-6(2)8(5)7(3)10/h4,9H,1-3H3
<b>InchiKey:</b>	VGZCKCJMYREIKA-UHFFFAOYSA-N
<b>Formula:</b>	C8H11NO
<b>SMILES:</b>	CC(=O)c1c(C)c[nH]c1C
<b>Mol. weight [g/mol]:</b>	137.18
<b>CAS:</b>	2386-25-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	1.352		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
rinpol	1298.00		NIST Webbook
rinpol	1298.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2386256&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2386256&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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