

# 1-[1,2,4]Triazol-1-ylethanone

<b>Other names:</b>	1-Acetyl-1H-1,2,4-triazole 1-Acetyl-1,2,4-triazole
<b>Inchi:</b>	InChI=1S/C4H5N3O/c1-4(8)7-3-5-2-6-7/h2-3H,1H3
<b>InchiKey:</b>	GLGDTYAVPSJOSQ-UHFFFAOYSA-N
<b>Formula:</b>	C4H5N3O
<b>SMILES:</b>	CC(=O)n1cncn1
<b>Mol. weight [g/mol]:</b>	111.10
<b>CAS:</b>	15625-88-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	-0.062		Crippen Method
mcvol	79.270	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15625884&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15625884&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>

## Legend

<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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