

# 3-Acetyl-2,5-dimethyl furan

<b>Other names:</b>	Ethanone, 1-(2,5-dimethyl-3-furanyl)- Furan, 3-acetyl-2,5-dimethyl 1-(2,5-dimethyl-3-furyl)ethan-1-one
<b>Inchi:</b>	InChI=1S/C8H10O2/c1-5-4-8(6(2)9)7(3)10-5/h4H,1-3H3
<b>InchiKey:</b>	KBSVBCHYXYXDAG-UHFFFAOYSA-N
<b>Formula:</b>	C8H10O2
<b>SMILES:</b>	CC(=O)c1cc(C)oc1C
<b>Mol. weight [g/mol]:</b>	138.16
<b>CAS:</b>	10599-70-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	2.099		Crippen Method
mcpol	111.560	ml/mol	McGowan Method
ripol	1103.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1118.00		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=C10599709&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10599709&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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  
**ripol:** Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/43-231-7/3-Acetyl-2-5-dimethyl-furan.pdf>

Generated by Cheméo on 2024-04-26 20:24:16.474236166 +0000 UTC m=+16452305.394813482.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.