

# Acetic acid, (1-methyl-4(1H)-pyridinylidene)-, methyl ester

<b>Inchi:</b>	InChI=1S/C9H11NO2/c1-10-5-3-8(4-6-10)7-9(11)12-2/h3-7H,1-2H3
<b>InchiKey:</b>	YLHYAULDARQGOT-UHFFFAOYSA-N
<b>Formula:</b>	C9H11NO2
<b>SMILES:</b>	COC(=O)C=C1C=CN(C)C=C1
<b>Mol. weight [g/mol]:</b>	165.19
<b>CAS:</b>	39998-22-6

## Physical Properties

Property code	Value	Unit	Source
ie	6.82 ± 0.02	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.059		Crippen Method
mcvol	131.330	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=C39998226&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C39998226&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>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/30-146-6/Acetic-acid-1-methyl-4-1H-pyridinylidene-methyl-ester.pdf>

Generated by Cheméo on 2024-04-18 22:31:29.970407868 +0000 UTC m=+15768738.890985180.

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