

# Methyl 2-pyridylacetate

<b>Other names:</b>	2-Pyridineacetic acid, methyl ester
<b>Inchi:</b>	InChI=1S/C8H9NO2/c1-11-8(10)6-7-4-2-3-5-9-7/h2-5H,6H2,1H3
<b>InchiKey:</b>	ORAKNQSHWMHCEY-UHFFFAOYSA-N
<b>Formula:</b>	C8H9NO2
<b>SMILES:</b>	COC(=O)Cc1ccccn1
<b>Mol. weight [g/mol]:</b>	151.16
<b>CAS:</b>	1658-42-0

## Physical Properties

Property code	Value	Unit	Source
ie	9.40 ± 0.02	eV	NIST Webbook
log10ws	-1.32		Crippen Method
logp	0.797		Crippen Method
mcvol	117.240	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	0.07	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1658420&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1658420&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>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
<b>tbrp:</b>	Boiling point at reduced pressure

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