

# Methyl 1-methylpyrrole-2-carboxylate

<b>Other names:</b>	2-(methoxycarbonyl)-1-methylpyrrole 2-methoxycarbonyl-N-methylpyrrole methyl 1-methyl-2-pyrrolecarboxylate methyl N-methylpyrrole-2-carboxylate
<b>Inchi:</b>	InChI=1S/C7H9NO2/c1-8-5-3-4-6(8)7(9)10-2/h3-5H,1-2H3
<b>InchiKey:</b>	APHVVGKYWHWFAQV-UHFFFAOYSA-N
<b>Formula:</b>	C7H9NO2
<b>SMILES:</b>	COC(=O)c1cccn1C
<b>Mol. weight [g/mol]:</b>	139.15
<b>CAS:</b>	37619-24-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	0.812		Crippen Method
mcvol	107.450	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	59.20	kJ/mol	298.15	Energetics and molecular structure of alkyl 1-methylpyrrolecarboxylates (alkyl = methyl or ethyl)

## 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=C37619242&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37619242&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>

## Legend

<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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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