

# Methylpyrazine-2-carboxylate

<b>Other names:</b>	Methyl pyrazinoate Pyrazinecarboxylic acid, methyl ester Methyl pyrazinecarboxylate Methyl 2-pyrazinecarboxylate Pyrazine-2-carboxylic acid, methyl ester Pyrazinoic acid methyl ester
<b>Inchi:</b>	InChI=1S/C6H6N2O2/c1-10-6(9)5-4-7-2-3-8-5/h2-4H,1H3
<b>InchiKey:</b>	TWIIIRMSFZNYMQE-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N2O2
<b>SMILES:</b>	<chem>COC(=O)c1cnccn1</chem>
<b>Mol. weight [g/mol]:</b>	138.12
<b>CAS:</b>	6164-79-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	0.263		Crippen Method
mcvol	99.040	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6164790&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6164790&amp;Units=SI</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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