

# 2-Furancarboxylic acid, 3-methyl-, methyl ester

<b>Other names:</b>	2-Furoic acid, 3-methyl-, methyl ester Methyl 3-methyl-2-furoate Methyl 3-methylfuroate
<b>Inchi:</b>	InChI=1S/C7H8O3/c1-5-3-4-10-6(5)7(8)9-2/h3-4H,1-2H3
<b>InchiKey:</b>	AQQYRDKMXXSIMP-UHFFFAOYSA-N
<b>Formula:</b>	C7H8O3
<b>SMILES:</b>	COC(=O)c1occc1C
<b>Mol. weight [g/mol]:</b>	140.14
<b>CAS:</b>	6141-57-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	1.375		Crippen Method
mcvol	103.340	ml/mol	McGowan Method

## 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=C6141577&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6141577&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>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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<https://www.chemeo.com/cid/12-290-6/2-Furancarboxylic-acid-3-methyl-methyl-ester.pdf>

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