

# 3-Furancarboxylic acid, 2,5-dimethyl-, methyl ester

<b>Other names:</b>	3-Furoic acid, 2,5-dimethyl-, methyl ester Methyl 2,5-dimethyl-3-furancarboxylate Methyl 2,5-dimethyl-3-furoate Methyl 2,5-dimethylfuran-3-carboxylate
<b>Inchi:</b>	InChI=1S/C8H10O3/c1-5-4-7(6(2)11-5)8(9)10-3/h4H,1-3H3
<b>InchiKey:</b>	MNFOIGQBJZVPCS-UHFFFAOYSA-N
<b>Formula:</b>	C8H10O3
<b>SMILES:</b>	<chem>COC(=O)c1cc(C)oc1C</chem>
<b>Mol. weight [g/mol]:</b>	154.16
<b>CAS:</b>	6148-34-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	1.683		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
tb	471.20	K	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6148341&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6148341&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tb:</b>	Normal Boiling Point Temperature

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