

# Methyl 3-amino-4-methylthiophene-2-carboxylate

<b>Other names:</b>	2-Thiophenecarboxylic acid, 3-amino-4-methyl-, methyl ester methyl 3-amino-4-methyl-2-thenoate
<b>Inchi:</b>	InChI=1S/C7H9NO2S/c1-4-3-11-6(5(4)8)7(9)10-2/h3H,8H2,1-2H3
<b>InchiKey:</b>	YICRPERKKBDRSP-UHFFFAOYSA-N
<b>Formula:</b>	C7H9NO2S
<b>SMILES:</b>	COC(=O)c1scc(C)c1N
<b>Mol. weight [g/mol]:</b>	171.22
<b>CAS:</b>	85006-31-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	1.425		Crippen Method
mcvol	123.800	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=C85006311&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85006311&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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