

# 3-Isoxazolecarboxylic acid, 5-methyl-, methyl ester

Other names:	Methyl 5-methylisoxazole-3-carboxylate
Inchi:	InChI=1S/C6H7NO3/c1-4-3-5(7-10-4)6(8)9-2/h3H,1-2H3
InchiKey:	MVHHQOCEOUNTID-UHFFFAOYSA-N
Formula:	C6H7NO3
SMILES:	COC(=O)c1cc(C)on1
Mol. weight [g/mol]:	141.12
CAS:	19788-35-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	0.770		Crippen Method
mcvol	99.230	ml/mol	McGowan Method

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19788353&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19788353&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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