

# Carbamic acid, 3-(5-nitro-2-furoyl)-, ethyl ester

<b>Inchi:</b>	InChI=1S/C8H9N3O6/c1-2-16-8(13)10-9-7(12)5-3-4-6(17-5)11(14)15/h3-4H,2H2,1H3,(H,
<b>InchiKey:</b>	MSOUQGDLZYBZQA-UHFFFAOYSA-N
<b>Formula:</b>	C8H9N3O6
<b>SMILES:</b>	CCOC(=O)NNC(=O)c1ccc([N+](=O)[O-])o1
<b>Mol. weight [g/mol]:</b>	243.17
<b>CAS:</b>	90223-46-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.06		Crippen Method
logp	0.579		Crippen Method
mcvol	156.380	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=C90223464&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C90223464&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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