

# 5-Imidazolic acid, 4-nitro-, methyl ester

<b>Other names:</b>	Imidazole-4-carboxylic acid, 5-nitro-, methyl ester
<b>Inchi:</b>	InChI=1S/C5H5N3O4/c1-12-5(9)3-4(8(10)11)7-2-6-3/h2H,1H3,(H,6,7)
<b>InchiKey:</b>	YGTWILAKCGDEML-UHFFFAOYSA-N
<b>Formula:</b>	C5H5N3O4
<b>SMILES:</b>	<chem>COC(=O)c1[nH]cnc1[N+](=O)[O-]</chem>
<b>Mol. weight [g/mol]:</b>	171.11
<b>CAS:</b>	20271-20-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	-0.377		Crippen Method
mcvol	106.670	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20271209&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20271209&amp;Units=SI</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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