

# Trigonelline

<b>Other names:</b>	Pyridinium, 3-carboxy-1-methyl-, hydroxide, inner salt Betaine nicotinate Caffearine Coffearin Coffearine Gynesine Trigenolline Betain nicotinate 3-Carboxy-1-methylpyridinium hydroxide inner salt N-Methylnicotinate N-Methylnicotinic acid N'-Methylnicotinic acid Nicotinic acid N-methylbetaine Trigonellin 1-methylpyridinio-3-carboxylate
<b>Inchi:</b>	InChI=1S/C7H7NO2/c1-8-4-2-3-6(5-8)7(9)10/h2-5H,1H3
<b>InchiKey:</b>	WWNNZCOKKKDOPX-UHFFFAOYSA-N
<b>Formula:</b>	C7H7NO2
<b>SMILES:</b>	<chem>C[n+]1cccc(C(=O)[O-])c1</chem>
<b>Mol. weight [g/mol]:</b>	137.14
<b>CAS:</b>	535-83-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.96		Crippen Method
logp	-1.125		Crippen Method
mcvol	103.150	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=C535831&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C535831&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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