

# 1-Methylpiperidine-3-carboxylic acid ethyl ester

<b>Other names:</b>	Ethyl 1-methyl-3-piperidinecarboxylate 3-Piperidinecarboxylic acid, 1-methyl-, ethyl ester Ethyl 1-methylnipecotate ethyl 1-methylpiperidine-3-carboxylate
<b>Inchi:</b>	InChI=1S/C9H17NO2/c1-3-12-9(11)8-5-4-6-10(2)7-8/h8H,3-7H2,1-2H3
<b>InchiKey:</b>	VFJJNMLPRDRTCO-UHFFFAOYSA-N
<b>Formula:</b>	C9H17NO2
<b>SMILES:</b>	CCOC(=O)C1CCCN(C)C1
<b>Mol. weight [g/mol]:</b>	171.24
<b>CAS:</b>	5166-67-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	0.891		Crippen Method
mcvol	144.230	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.70	K	1.50	NIST Webbook

## 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=C5166676&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5166676&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
<b>tbrp:</b>	Boiling point at reduced pressure

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