

# 2-Pyrrolidone-5-carboxylic acid, N-methyl, methyl ester

Inchi:	InChI=1S/C7H11NO3/c1-8-5(7(10)11-2)3-4-6(8)9/h5H,3-4H2,1-2H3
InchiKey:	ABAOXDQXQHQRFA-UHFFFAOYSA-N
Formula:	C7H11NO3
SMILES:	COC(=O)C1CCC(=O)N1C
Mol. weight [g/mol]:	157.17

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.03		Crippen Method
logp	-0.220		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
rinpola	1163.30		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
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=U333168&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333168&amp;Units=SI</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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