

# Isonipecotic acid, N-methoxycarbonyl-, propyl ester

<b>Inchi:</b>	InChI=1S/C11H19NO4/c1-3-8-16-10(13)9-4-6-12(7-5-9)11(14)15-2/h9H,3-8H2,1-2H3
<b>InchiKey:</b>	KJBBKJFLIWGYMY-UHFFFAOYSA-N
<b>Formula:</b>	C11H19NO4
<b>SMILES:</b>	CCCOC(=O)C1CCN(C(=O)OC)CC1
<b>Mol. weight [g/mol]:</b>	229.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	1.418		Crippen Method
mcvol	179.850	ml/mol	McGowan Method
rinpola	1703.00		NIST Webbook

## Sources

<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=U322017&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U322017&amp;Units=SI</a>
<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>

## 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>rinpola:</b>	Non-polar retention indices

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