

# Isonipecotic acid, N-methoxycarbonyl-, isobutyl ester

<b>Inchi:</b>	InChI=1S/C12H21NO4/c1-9(2)8-17-11(14)10-4-6-13(7-5-10)12(15)16-3/h9-10H,4-8H2,1-
<b>InchiKey:</b>	YZNUVAVHQISUCK-UHFFFAOYSA-N
<b>Formula:</b>	C12H21NO4
<b>SMILES:</b>	COC(=O)N1CCC(C(=O)OCC(C)C)CC1
<b>Mol. weight [g/mol]:</b>	243.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	1.664		Crippen Method
mcvol	193.940	ml/mol	McGowan Method
rinpol	1762.00		NIST Webbook

## 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=U322018&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U322018&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
<b>rinpol:</b>	Non-polar retention indices

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