

# Isonipecotic acid, N-(3-chloropropionyl)-, ethyl ester

<b>Inchi:</b>	InChI=1S/C11H18ClNO3/c1-2-16-11(15)9-4-7-13(8-5-9)10(14)3-6-12/h9H,2-8H2,1H3
<b>InchiKey:</b>	RQAVOJRSNJZSIB-UHFFFAOYSA-N
<b>Formula:</b>	C11H18ClNO3
<b>SMILES:</b>	CCOC(=O)C1CCN(C(=O)CCCl)CC1
<b>Mol. weight [g/mol]:</b>	247.72

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	1.417		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
rinpola	1876.00		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=U360941&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360941&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>
<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>rinpola:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/68-040-2/Isonipecotic-acid-N-3-chloropropionyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-24 01:42:55.145067195 +0000 UTC m=+16212224.065644510.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.