

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

<b>Inchi:</b>	InChI=1S/C15H26ClNO3/c1-12(2)4-3-11-20-15(19)13-6-9-17(10-7-13)14(18)5-8-16/h12-
<b>InchiKey:</b>	AXUCIFXVSRNPAX-UHFFFAOYSA-N
<b>Formula:</b>	C15H26ClNO3
<b>SMILES:</b>	CC(C)CCCOC(=O)C1CCN(C(=O)CCCl)CC1
<b>Mol. weight [g/mol]:</b>	303.82

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	2.833		Crippen Method
mcpol	242.580	ml/mol	McGowan Method
rinpol	2265.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U360945&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360945&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>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcpol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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