

# Isonipecotic acid, N-(5-chlorovaleryl)-, propyl ester

<b>Inchi:</b>	InChI=1S/C14H24ClNO3/c1-2-11-19-14(18)12-6-9-16(10-7-12)13(17)5-3-4-8-15/h12H,2-
<b>InchiKey:</b>	YKKSPCSAJXJEDL-UHFFFAOYSA-N
<b>Formula:</b>	C14H24ClNO3
<b>SMILES:</b>	CCCOC(=O)C1CCN(C(=O)CCCCCl)CC1
<b>Mol. weight [g/mol]:</b>	289.80

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	2.587		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
rinpola	2340.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361003&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361003&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.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>

## 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.cheméo.com/cid/45-702-2/Isonipecotic-acid-N-5-chlorovaleryl-propyl-ester.pdf>

Generated by Cheméo on 2024-04-29 13:28:58.246034405 +0000 UTC m=+16686587.166611722.

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