

# L-Proline, N-(5-chlorovaleryl)-, heptyl ester

<b>Inchi:</b>	InChI=1S/C17H30ClNO3/c1-2-3-4-5-8-14-22-17(21)15-10-9-13-19(15)16(20)11-6-7-12-1
<b>InchiKey:</b>	LGJOYYRDFUUOPB-UHFFFAOYSA-N
<b>Formula:</b>	C17H30ClNO3
<b>SMILES:</b>	CCCCCCCOC(=O)C1CCCN1C(=O)CCCCCI
<b>Mol. weight [g/mol]:</b>	331.88

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	3.900		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U346236&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346236&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>
<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>

## 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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