

# L-Proline, N-(3-chloro-2-fluorobenzoyl)-, nonyl ester

Inchi:	InChI=1S/C21H29ClFNO3/c1-2-3-4-5-6-7-8-15-27-21(26)18-13-10-14-24(18)20(25)16-17
InchiKey:	MOFLICLOEGQPMA-UHFFFAOYSA-N
Formula:	C21H29ClFNO3
SMILES:	CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]:	397.91

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Crippen Method
logp	5.377		Crippen Method
mcvol	305.130	ml/mol	McGowan Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U345941&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345941&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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