

# I-Proline, N-(4-fluorobenzoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C13H14FNO3/c1-18-13(17)11-3-2-8-15(11)12(16)9-4-6-10(14)7-5-9/h4-7,11H,
<b>InchiKey:</b>	QVPGJZSAXQQSQB-UHFFFAOYSA-N
<b>Formula:</b>	C13H14FNO3
<b>SMILES:</b>	COC(=O)C1CCCN1C(=O)c1ccc(F)cc1
<b>Mol. weight [g/mol]:</b>	251.25

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.603		Crippen Method
mcvol	180.170	ml/mol	McGowan Method
rinpol	1880.00		NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299606&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299606&amp;Units=SI</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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