l-Proline, N-(4-fluorobenzoyl)-, methyl ester

Inchi:	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,
InchiKey:	QVPGJZSAXQQSQB-UHFFFAOYSA-N
Formula:	C13H14FNO3
SMILES:	COC(=O)C1CCCN1C(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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