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

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299606&Units=SI

Legend

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