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

Inchi: InChI=1S/C15H17ClFNO3/c1-2-9-21-15(20)12-7-4-8-18(12)14(19)10-5-3-6-11(16)13(10)
InchiKey: JDHDXZGGNRDKIM-UHFFFAOYSA-N
Formula: C15H17ClFNO3
SMILES: CCCOC(=O)C1CCCN1C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 313.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	3.037		Crippen Method
mcvol	220.590	ml/mol	McGowan Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345935&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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