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

Inchi: InChI=1S/C14H15ClFNO3/c1-2-20-14(19)11-7-4-8-17(11)13(18)9-5-3-6-10(15)12(9)16/h

InchiKey: UCUHTVIRBRTRDO-UHFFFAOYSA-N

Formula: C14H15ClFNO3

SMILES: CCOC(=O)C1CCCN1C(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 299.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.647		Crippen Method
mcvol	206.500	ml/mol	McGowan Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook

Sources

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=U345934&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.