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

Inchi: InChI=1S/C23H33ClFNO3/c1-2-3-4-5-6-7-8-9-10-17-29-23(28)20-15-12-16-26(20)22(27)
InchiKey: BTQHZWHIICVNLE-UHFFFAOYSA-N
Formula: C23H33ClFNO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 425.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.36		Crippen Method
logp	6.158		Crippen Method
mcvol	333.310	ml/mol	McGowan Method
rinpol	3113.00		NIST Webbook
rinpol	3113.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345943&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.