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

Inchi: InChI=1S/C26H39ClFNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-32-26(31)23-18-15-19-29(

InchiKey: SYPUXDNROOPSOY-UHFFFAOYSA-N

Formula: C26H39ClFNO3

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

Mol. weight [g/mol]: 468.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.62		Crippen Method
logp	7.328		Crippen Method
mcvol	375.580	ml/mol	McGowan Method
rinpol	3441.00		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=U345945&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