

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

Inchi: InChI=1S/C24H35ClFNO3/c1-2-3-4-5-6-7-8-9-10-11-18-30-24(29)21-16-13-17-27(21)23(29)22-12
InchiKey: JXDJBFIMURVUJO-UHFFFAOYSA-N
Formula: C₂₄H₃₅ClFNO₃
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 439.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.78		Crippen Method
logp	6.548		Crippen Method
mcvol	347.400	ml/mol	McGowan Method
rinpol	3230.00		NIST Webbook
rinpol	3230.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345944&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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