

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

Inchi: InChI=1S/C18H23ClFNO3/c1-12(2)6-5-11-24-18(23)15-9-4-10-21(15)17(22)13-7-3-8-14(18)
InchiKey: RARLSDHYZZCPGD-UHFFFAOYSA-N
Formula: C18H23ClFNO3
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 355.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	4.063		Crippen Method
mcvol	262.860	ml/mol	McGowan Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		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=U345947&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.chemeo.com/cid/115-979-8/L-Proline-N-3-chloro-2-fluorobenzoyl-isohexyl-ester.pdf>

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