

L-Proline, N-(2-fluorobenzoyl)-, propyl ester

Inchi: InChI=1S/C15H18FNO3/c1-2-10-20-15(19)13-8-5-9-17(13)14(18)11-6-3-4-7-12(11)16/h3
InchiKey: AUOQPPVLKKUODF-UHFFFAOYSA-N
Formula: C15H18FNO3
SMILES: CCCOC(=O)C1CCCN1C(=O)c1ccccc1F
Mol. weight [g/mol]: 279.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	2.383		Crippen Method
mcvol	208.350	ml/mol	McGowan Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U346092&Units=SI>

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/124-221-8/L-Proline-N-2-fluorobenzoyl-propyl-ester.pdf>

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