

L-Proline, N-(4-chlorobenzoyl)-, propyl ester

Inchi: InChI=1S/C15H18ClNO3/c1-2-10-20-15(19)13-4-3-9-17(13)14(18)11-5-7-12(16)8-6-11/h
InchiKey: JEMHGWYSYLKGC-F-UHFFFAOYSA-N
Formula: C₁₅H₁₈ClNO₃
SMILES: CCCOC(=O)C1CCCN1C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 295.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.898		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346145&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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