

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

Inchi: InChI=1S/C17H22ClNO3/c1-2-3-4-12-22-17(21)15-6-5-11-19(15)16(20)13-7-9-14(18)10-
InchiKey: HPOZMSPTBQFYRQ-UHFFFAOYSA-N
Formula: C17H22ClNO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 323.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	3.678		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346147&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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