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

Inchi: InChI=1S/C14H16ClNO3/c1-2-19-14(18)12-4-3-9-16(12)13(17)10-5-7-11(15)8-6-10/h5-8
InchiKey: JSFFSEZTGFQFHU-UHFFFAOYSA-N
Formula: C14H16ClNO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 281.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.508		Crippen Method
mcvol	204.730	ml/mol	McGowan Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U346144&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.