L-Proline, N-(2-chlorobenzoyl)-, butyl ester

Inchi: InChI=1S/C16H20ClNO3/c1-2-3-11-21-16(20)14-9-6-10-18(14)15(19)12-7-4-5-8-13(12)1
InchiKey: IEJRXSXRCPTAPG-UHFFFAOYSA-N
Formula: C16H20ClNO3
SMILES: CCCCOC(=O)C1CCCN1C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 309.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	3.288		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346051&Units=SI
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

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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