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

Inchi: InChI=1S/C20H28ClNO3/c1-2-3-4-5-6-9-15-25-20(24)18-13-10-14-22(18)19(23)16-11-7-
InchiKey: AONMDUFRANCOFF-UHFFFAOYSA-N
Formula: C20H28ClNO3
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 365.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	4.848		Crippen Method
mcvol	289.270	ml/mol	McGowan Method
rinpol	2773.00		NIST Webbook
rinpol	2773.00		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=U346056&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.