

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

Inchi: InChI=1S/C21H30ClNO3/c1-2-3-4-5-6-7-10-16-26-21(25)19-14-11-15-23(19)20(24)17-12
InchiKey: IXHMJTTWBSQCEY-UHFFFAOYSA-N
Formula: C21H30ClNO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 379.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	5.238		Crippen Method
mcvol	303.360	ml/mol	McGowan Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346057&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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