

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

Inchi:	InChI=1S/C18H24ClNO3/c1-13(2)5-4-12-23-18(22)16-6-3-11-20(16)17(21)14-7-9-15(19)
InchiKey:	CCYBGFPWKNNXEG-UHFFFAOYSA-N
Formula:	C18H24ClNO3
SMILES:	CC(C)CCCOC(=O)C1CCCN1C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	337.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	3.924		Crippen Method
mcvol	261.090	ml/mol	McGowan Method
rinpol	2568.00		NIST Webbook
rinpol	2568.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346148&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

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