

L-Proline, N-(3-chloropropionyl)-, isobutyl ester

Inchi:	InChI=1S/C12H20ClNO3/c1-9(2)8-17-12(16)10-4-3-7-14(10)11(15)5-6-13/h9-10H,3-8H2
InchiKey:	HSAQMHLAXYBHCE-UHFFFAOYSA-N
Formula:	C12H20ClNO3
SMILES:	CC(C)COC(=O)C1CCCN1C(=O)CCCI
Mol. weight [g/mol]:	261.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.805		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
rinpol	1958.00		NIST Webbook
rinpol	1958.00		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=U346334&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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