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

Inchi: InChI=1S/C11H18ClNO3/c1-2-8-16-11(15)9-4-3-7-13(9)10(14)5-6-12/h9H,2-8H2,1H3
InchiKey: SJQMJJDJKCGHFB-UHFFFAOYSA-N
Formula: C11H18ClNO3
SMILES: CCCOC(=O)C1CCCN1C(=O)CCCl
Mol. weight [g/mol]: 247.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	1.560		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346333&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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