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

Inchi: InChI=1S/C13H22ClNO3/c1-2-3-4-10-18-13(17)11-6-5-9-15(11)12(16)7-8-14/h11H,2-10H
InchiKey: MWZGLEUBCHZKSZ-UHFFFAOYSA-N
Formula: C13H22ClNO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)CCCl
Mol. weight [g/mol]: 275.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	2.340		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346336&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.