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

Inchi: InChI=1S/C10H16ClNO3/c1-2-15-10(14)8-4-3-7-12(8)9(13)5-6-11/h8H,2-7H2,1H3
InchiKey: DZFYSLIZVURFFK-UHFFFAOYSA-N
Formula: C10H16ClNO3
SMILES: CCOC(=O)C1CCCN1C(=O)CCCl
Mol. weight [g/mol]: 233.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	1.169		Crippen Method
mcvol	172.130	ml/mol	McGowan Method
rinpol	1822.00		NIST Webbook
rinpol	1822.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346332&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.