

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

Inchi: InChI=1S/C12H20ClNO3/c1-2-3-9-17-12(16)10-5-4-8-14(10)11(15)6-7-13/h10H,2-9H2,1H
InchiKey: PNFBOCROUZPUGK-UHFFFAOYSA-N
Formula: C12H20ClNO3
SMILES: CCCOC(=O)C1CCCN1C(=O)CCCl
Mol. weight [g/mol]: 261.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	1.950		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346335&Units=SI>
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>

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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