L-Proline, N-(5-chlorovaleryl)-, butyl ester

Inchi: InChI=1S/C14H24ClNO3/c1-2-3-11-19-14(18)12-7-6-10-16(12)13(17)8-4-5-9-15/h12H,2-
InchiKey: UPDJYFPWRJMKBO-UHFFFAOYSA-N
Formula: C14H24ClNO3
SMILES: CCCCOC(=O)C1CCCN1C(=O)CCCCCl
Mol. weight [g/mol]: 289.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.730		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346233&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.