

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

Inchi: InChI=1S/C16H28ClNO3/c1-2-3-4-7-13-21-16(20)14-9-8-12-18(14)15(19)10-5-6-11-17/h
InchiKey: GRHTVAACXZRWCD-UHFFFAOYSA-N
Formula: C16H28ClNO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)CCCCCI
Mol. weight [g/mol]: 317.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	3.510		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346235&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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