

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

Inchi: InChI=1S/C14H24ClNO3/c1-2-3-4-5-11-19-14(18)12-7-6-10-16(12)13(17)8-9-15/h12H,2-
InchiKey: OMMKXLPQKPZUGX-UHFFFAOYSA-N
Formula: C14H24ClNO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)CCCl
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
rinsol	2192.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346337&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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<https://www.chemeo.com/cid/116-337-9/L-Proline-N-3-chloropropionyl-hexyl-ester.pdf>

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