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

Inchi: InChI=1S/C19H34ClNO3/c1-2-3-4-5-6-7-8-9-10-16-24-19(23)17-12-11-15-21(17)18(22)1

InchiKey: WRTASDDWXNAKLU-UHFFFAOYSA-N

Formula: C19H34ClNO3

SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)CCCl

Mol. weight [g/mol]: 359.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	4.680		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346338&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

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