L-Proline, N-(cyclopropylcarbonyl)-, hexyl ester

Inchi: InChI=1S/C15H25NO3/c1-2-3-4-5-11-19-15(18)13-7-6-10-16(13)14(17)12-8-9-12/h12-13

InchiKey: CHCIWCVMRVWINA-UHFFFAOYSA-N

Formula: C15H25NO3

SMILES: CCCCCCOC(=O)C1CCCN1C(=O)C1CC1

Mol. weight [g/mol]: 267.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	2.511		Crippen Method
mcvol	219.480	ml/mol	McGowan Method
rinpol	2099.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346313&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