

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

Inchi:	InChI=1S/C12H19NO3/c1-2-8-16-12(15)10-4-3-7-13(10)11(14)9-5-6-9/h9-10H,2-8H2,1H
InchiKey:	VTFCIKFSHHPUDA-UHFFFAOYSA-N
Formula:	C12H19NO3
SMILES:	CCCOC(=O)C1CCCN1C(=O)C1CC1
Mol. weight [g/mol]:	225.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	1.341		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
rinpol	1798.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U346309&Units=SI

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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<https://www.chemeo.com/cid/85-298-8/L-Proline-N-cyclopropylcarbonyl-propyl-ester.pdf>

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