

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

Inchi:	InChI=1S/C13H21NO3/c1-2-3-9-17-13(16)11-5-4-8-14(11)12(15)10-6-7-10/h10-11H,2-9H
InchiKey:	GIZCRHMTXMESDS-UHFFFAOYSA-N
Formula:	C13H21NO3
SMILES:	CCCCOC(=O)C1CCCN1C(=O)C1CC1
Mol. weight [g/mol]:	239.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.731		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346310&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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