

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

Inchi:	InChI=1S/C15H25NO3/c1-11(2)5-4-10-19-15(18)13-6-3-9-16(13)14(17)12-7-8-12/h11-13
InchiKey:	ZTSUPMZBGVUPSG-UHFFFAOYSA-N
Formula:	C15H25NO3
SMILES:	CC(C)CCCOC(=O)C1CCCN1C(=O)C1CC1
Mol. weight [g/mol]:	267.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	2.367		Crippen Method
mcvol	219.480	ml/mol	McGowan Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346312&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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