

L-Proline, N-(cyclohexanecarbonyl)-, pentyl ester

Inchi:	InChI=1S/C17H29NO3/c1-2-3-7-13-21-17(20)15-11-8-12-18(15)16(19)14-9-5-4-6-10-14/
InchiKey:	NUNBXPMMGGQPBDK-UHFFFAOYSA-N
Formula:	C17H29NO3
SMILES:	CCCCCOC(=O)C1CCCN1C(=O)C1CCCCC1
Mol. weight [g/mol]:	295.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	3.291		Crippen Method
mcvol	247.660	ml/mol	McGowan Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346180&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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