

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

Inchi:	InChI=1S/C18H31NO3/c1-14(2)8-7-13-22-18(21)16-11-6-12-19(16)17(20)15-9-4-3-5-10-
InchiKey:	HNKRMTIURNRWSB-UHFFFAOYSA-N
Formula:	C18H31NO3
SMILES:	CC(C)CCCOC(=O)C1CCCN1C(=O)C1CCCCC1
Mol. weight [g/mol]:	309.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.537		Crippen Method
mcvol	261.750	ml/mol	McGowan Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346181&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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