

L-Proline, N-(3-cyclopentylpropionyl)-, isohexyl ester

Inchi:	InChI=1S/C19H33NO3/c1-15(2)7-6-14-23-19(22)17-10-5-13-20(17)18(21)12-11-16-8-3-4
InchiKey:	DZRFBKWQUHXYCPS-UHFFFAOYSA-N
Formula:	C19H33NO3
SMILES:	CC(C)CCCOC(=O)C1CCCN1C(=O)CCC1CCCC1
Mol. weight [g/mol]:	323.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	3.927		Crippen Method
mcvol	275.840	ml/mol	McGowan Method
rinpol	2465.00		NIST Webbook
rinpol	2465.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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