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: DZRFKWQUHXYCPS-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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346411&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.