

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

Inchi: InChI=1S/C19H33NO3/c1-2-3-4-7-15-23-19(22)17-11-8-14-20(17)18(21)13-12-16-9-5-6-
InchiKey: LLGAOBVLIRHCJS-UHFFFAOYSA-N
Formula: C19H33NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)CCC1CCCC1
Mol. weight [g/mol]: 323.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.071		Crippen Method
mcvol	275.840	ml/mol	McGowan Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346412&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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