l-Proline, N-(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C14H23NO3/c1-18-14(17)12-7-4-10-15(12)13(16)9-8-11-5-2-3-6-11/h11-12H,2

InchiKey: VGIIPOBEENRBLB-UHFFFAOYSA-N

Formula: C14H23NO3

SMILES: COC(=O)C1CCCN1C(=O)CCC1CCCC1

Mol. weight [g/mol]: 253.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	2.121		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299654&Units=SI

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

Crippen Method: https://www.chemeo.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

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