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

Inchi: InChI=1S/C17H29NO3/c1-2-3-13-21-17(20)15-9-6-12-18(15)16(19)11-10-14-7-4-5-8-14/h
InchiKey: QKQWYIYQKQXTNZ-UHFFFAOYSA-N
Formula: C17H29NO3
SMILES: CCCCOC(=O)C1CCCN1C(=O)CCC1CCCC1
Mol. weight [g/mol]: 295.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	3.291		Crippen Method
mcvol	247.660	ml/mol	McGowan Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346409&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.