L-Proline, N-(3-phenylpropionyl)-, propyl ester

Inchi: InChI=1S/C17H23NO3/c1-2-13-21-17(20)15-9-6-12-18(15)16(19)11-10-14-7-4-3-5-8-14/h
InchiKey: ZEWIWNCZRUMAPH-UHFFFAOYSA-N
Formula: C17H23NO3
SMILES: CCCOC(=O)C1CCCN1C(=O)CCc1ccccc1
Mol. weight [g/mol]: 289.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.563		Crippen Method
mcvol	234.760	ml/mol	McGowan Method
rinpol	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346382&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.