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

Inchi: InChI=1S/C18H25NO3/c1-14(2)13-22-18(21)16-9-6-12-19(16)17(20)11-10-15-7-4-3-5-8-
InchiKey: VERBDNDRULKCDH-UHFFFAOYSA-N
Formula: C18H25NO3
SMILES: CC(C)COC(=O)C1CCCN1C(=O)CCc1ccccc1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	2.809		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346383&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.