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

Inchi: InChI=1S/C21H31NO3/c1-2-3-4-5-9-17-25-21(24)19-13-10-16-22(19)20(23)15-14-18-11-
InchiKey: QUWQYPUHAZSXNG-UHFFFAOYSA-N
Formula: C21H31NO3
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)CCc1ccccc1
Mol. weight [g/mol]: 345.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	4.124		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
rinpol	2743.00		NIST Webbook
rinpol	2743.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346388&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.