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

Inchi: InChI=1S/C20H29NO3/c1-16(2)8-7-15-24-20(23)18-11-6-14-21(18)19(22)13-12-17-9-4-3

InchiKey: JPJMDJPKTAACJZ-UHFFFAOYSA-N

Formula: C20H29NO3

SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)CCc1ccccc1

Mol. weight [g/mol]: 331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.590		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346386&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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