L-Proline, N-(phenylacetyl)-, heptyl ester

Inchi: InChI=1S/C20H29NO3/c1-2-3-4-5-9-15-24-20(23)18-13-10-14-21(18)19(22)16-17-11-7-6
InchiKey: MLKXXNMBKBQJLZ-UHFFFAOYSA-N
Formula: C20H29NO3
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)Cc1ccccc1
Mol. weight [g/mol]: 331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	3.734		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U346194&Units=SI

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.