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

Inchi: InChI=1S/C16H21NO3/c1-2-11-20-16(19)14-9-6-10-17(14)15(18)12-13-7-4-3-5-8-13/h3-5
InchiKey: PQOPDPJUQMLYBL-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: CCCOC(=O)C1CCCN1C(=O)Cc1ccccc1
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	2.173		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
rinpol	2237.00		NIST Webbook
rinpol	2237.00		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=U346190&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.