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

Inchi: InChI=1S/C18H25NO3/c1-2-3-7-13-22-18(21)16-11-8-12-19(16)17(20)14-15-9-5-4-6-10-
InchiKey: HTZALULWXUKBDX-UHFFFAOYSA-N
Formula: C18H25NO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)Cc1ccccc1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	2.954		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		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=U346191&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.