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

Inchi: InChI=1S/C19H27NO3/c1-15(2)8-7-13-23-19(22)17-11-6-12-20(17)18(21)14-16-9-4-3-5-
InchiKey: ACCZYRYHDCRGOU-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)Cc1ccccc1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	3.199		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346192&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.