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

Inchi: InChI=1S/C27H43NO3/c1-2-3-4-5-6-7-8-9-10-11-12-16-22-31-27(30)25-20-17-21-28(25)
InchiKey: KGHQQQPDIRZDMU-UHFFFAOYSA-N
Formula: C27H43NO3
SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)Cc1ccccc1
Mol. weight [g/mol]: 429.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.44		Crippen Method
logp	6.464		Crippen Method
mcvol	375.660	ml/mol	McGowan Method
rinpol	3387.00		NIST Webbook
rinpol	3387.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346200&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

Latest version available from:
https://www.chemeo.com/cid/94-790-1/L-Proline-N-phenylacetyl-tetradecyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:52:35.926295582 +0000 UTC m=+3286018.563264831.

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