L-Proline, N-(3-methoxybenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C27H43NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-21-32-27(30)25-19-16-20-28(25
InchiKey: CZUSGKBAYGMSHY-UHFFFAOYSA-N
Formula: C27H43NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 445.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.72		Crippen Method
logp	6.544		Crippen Method
mcvol	381.530	ml/mol	McGowan Method
rinpol	3523.00		NIST Webbook
rinpol	3523.00		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=U346175&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.