

L-Proline, N-(3-phenylpropionyl)-, dodecyl ester

Inchi:	InChI=1S/C26H41NO3/c1-2-3-4-5-6-7-8-9-10-14-22-30-26(29)24-18-15-21-27(24)25(28)
InchiKey:	RLDVFDZRJKOSIF-UHFFFAOYSA-N
Formula:	C26H41NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)CCc1cccc1
Mol. weight [g/mol]:	415.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.02		Crippen Method
logp	6.074		Crippen Method
mcvol	361.570	ml/mol	McGowan Method
rinpol	3285.00		NIST Webbook
rinpol	3285.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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