

L-Proline, N-(cyclohexanecarbonyl)-, dodecyl ester

Inchi:	InChI=1S/C24H43NO3/c1-2-3-4-5-6-7-8-9-10-14-20-28-24(27)22-18-15-19-25(22)23(26)
InchiKey:	UPWAHSKDFMVMKE-UHFFFAOYSA-N
Formula:	C24H43NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C1CCCCC1
Mol. weight [g/mol]:	393.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.74		Crippen Method
logp	6.022		Crippen Method
mcvol	346.290	ml/mol	McGowan Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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