

L-Proline, N-(3-methylbenzoyl)-, hexadecyl ester

Inchi:	InChI=1S/C29H47NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-33-29(32)27-21-18-22
InchiKey:	KHNLZNBIBQOBQTD-UHFFFAOYSA-N
Formula:	C29H47NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]:	457.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.91		Crippen Method
logp	7.624		Crippen Method
mcvol	403.840	ml/mol	McGowan Method
rinpol	3603.00		NIST Webbook
rinpol	3603.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346265&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

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