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

Inchi:	InChI=1S/C21H31NO3/c1-3-4-5-6-7-8-15-25-21(24)19-13-10-14-22(19)20(23)18-12-9-11
InchiKey:	FBYACADBIOUKIO-UHFFFAOYSA-N
Formula:	C21H31NO3
SMILES:	CCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]:	345.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	4.503		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
rinpol	2728.00		NIST Webbook
rinpol	2728.00		NIST Webbook

Sources

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=U346258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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