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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346258&Units=SI
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

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.