

L-Proline, N-(4-butylbenzoyl)-, octyl ester

Inchi: InChI=1S/C24H37NO3/c1-3-5-7-8-9-10-19-28-24(27)22-13-11-18-25(22)23(26)21-16-14-
InchiKey: JSRJEDFAJUEWGD-UHFFFAOYSA-N
Formula: C24H37NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 387.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	5.538		Crippen Method
mcvol	333.390	ml/mol	McGowan Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346274&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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