

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

Inchi: InChI=1S/C18H25NO3/c1-3-4-5-12-22-18(21)16-10-7-11-19(16)17(20)15-9-6-8-14(2)13-
InchiKey: SGMATPPCTBIGBH-UHFFFAOYSA-N
Formula: C18H25NO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	3.333		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346254&Units=SI>
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>

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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