

L-Proline, N-(3-methoxybenzoyl)-, butyl ester

Inchi: InChI=1S/C17H23NO4/c1-3-4-11-22-17(20)15-9-6-10-18(15)16(19)13-7-5-8-14(12-13)21
InchiKey: OLGWMAIFJFDZHV-UHFFFAOYSA-N
Formula: C17H23NO4
SMILES: CCCOC(=O)C1CCCN1C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 305.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	2.643		Crippen Method
mcvol	240.630	ml/mol	McGowan Method
rinpol	2479.00		NIST Webbook
rinpol	2479.00		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=U346169&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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