

L-Proline, N-(3-bromobenzoyl)-, ethyl ester

Inchi: InChI=1S/C14H16BrNO3/c1-2-19-14(18)12-7-4-8-16(12)13(17)10-5-3-6-11(15)9-10/h3,5
InchiKey: FZOZQNZYJHJQDL-UHFFFAOYSA-N
Formula: C14H16BrNO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 326.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	2.617		Crippen Method
mcvol	209.990	ml/mol	McGowan Method
rinpol	2312.00		NIST Webbook
rinpol	2312.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346137&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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<https://www.chemeo.com/cid/115-914-9/L-Proline-N-3-bromobenzoyl-ethyl-ester.pdf>

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