

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

Inchi: InChI=1S/C16H20BrNO3/c1-11(2)10-21-16(20)14-7-4-8-18(14)15(19)12-5-3-6-13(17)9-1
InchiKey: MEZXJFZFKLAFKD-UHFFFAOYSA-N
Formula: C16H20BrNO3
SMILES: CC(C)COC(=O)C1CCCN1C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 354.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.253		Crippen Method
mcvol	238.170	ml/mol	McGowan Method
rinpol	2461.00		NIST Webbook
rinpol	2461.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346139&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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