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Typical Product Specifications & Properties

tert-Butyl 3-(4-bromophenyl)pyrrolidine-1-carboxylate

CAS Number: : 1467060-28-1

Specifications	Limits
Chemical Structure	 chemicalStructure-tert-butyl-3-4-bromophenyl-pyrrolidine-1-carboxylate
CAS-like Style IUPAC Name	3-(4-bromophenyl)-1-pyrrolidinecarboxylic acid tert-butyl ester
Markup IUPAC Name	<l>tert</l>-butyl 3-(4-bromophenyl)pyrrolidine-1-carboxylate
Preferred IUPAC Name	tert-butyl 3-(4-bromophenyl)pyrrolidine-1-carboxylate
Systematic IUPAC Name	tert-butyl 3-(4-bromophenyl)pyrrolidine-1-carboxylate
Traditional IUPAC Name	3-(4-bromophenyl)pyrrolidine-1-carboxylic acid tert-butyl ester
Standard InChI	InChI=1S/C15H20BrNO2/c1-15(2,3)19-14(18)17-9-8-12(10-17)11-4-6-13(16)7-5-11/h4-7,12H,8-10H2,1-3H3
Standard InChIKey	NFTKVQYDQFSNHQ-UHFFFAOYSA-N
XLogP3-AA Log P	3.7
Exact Mass	325.06774
Molecular Weight	326.23



CC(C)(C)OC(=O)N1CC(C1)C2=CC=C(C=C2)Br

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Specifications	Limits
Isomeric SMILES	<chem>CC(C)(C)OC(=O)N1CCC(C1)C2=CC=C(C=C2)Br</chem>
Polar Surface Area Topological	29.5
Monoisotopic Weight	325.06774
Molecular Formula	C15H20BrNO2
Molecular weight	
Canonicalized Compound	1
Compound Complexity	319
Hydrogen Bond Acceptor Count	2
Hydrogen Bond Donor Count	
Rotatable Bond Count	3
Specifications	Limits

Allowed IUPAC Name

tert-butyl 3-(4-bromophenyl)pyrrolidine-1-carboxylate

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