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Typical Product Specifications & Properties

tert-butyl 4,4-difluoropiperidine-1-carboxylate

CAS Number: : 281652-10-6

Specifications	Limits
Chemical Structure	 chemicalStructure-tert-butyl-4-4-difluoropiperidine-1-carboxylate
Allowed IUPAC Name	tert-butyl 4,4-difluoropiperidine-1-carboxylate
CAS-like Style IUPAC Name	4,4-difluoro-1-piperidinecarboxylic acid tert-butyl ester
Markup IUPAC Name	<l>tert</l>-butyl 4,4-difluoropiperidine-1-carboxylate
Preferred IUPAC Name	tert-butyl 4,4-difluoropiperidine-1-carboxylate
Systematic IUPAC Name	tert-butyl 4,4-bis(fluoranyl)piperidine-1-carboxylate
Traditional IUPAC Name	4,4-difluoropiperidine-1-carboxylic acid tert-butyl ester
Standard InChI	InChI=1S/C10H17F2NO2/c1-9(2,3)15-8(14)13-6-4-10(11,12)5-7-13/h4-7H2,1-3H3
Standard InChIKey	HHBBBPZ PEBZ LII-UHFFFAOYSA-N
XLogP3-AA Log P	2.3
Exact Mass	221.12273511
Molecular Weight	221.24



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Specifications	Limits
Canonical SMILES	<chem>CC(C)(C)OC(=O)N1CCC(CC1)(F)F</chem>
Isomeric SMILES	<chem>CC(C)(C)OC(=O)N1CCC(CC1)(F)F</chem>
Polar Surface Area Topological	29.5
Monoisotopic Weight	221.12273511
Molecular Formula	C10H17F2NO2
Molecular weight	
Canonicalized Compound	1
Compound Complexity	238
Hydrogen Bond Acceptor Count	4
Hydrogen Bond Donor Count	
Rotatable Bond Count	2



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