Typical Product Specifications & Properties

4-CarBoxy-3-fluoroBenzeneBoronicacid,pinacole

CAS Number: : 867256-77-7

Specifications	Limits
Isomeric SMILES	B1(OC(C(O1)(C)C)(C)C)C2=CC(=C(C=C2)C(=O)O)F
Polar Surface Area Topological	55.8
Monolsotopic Weight	266.1125673
Molecular Formula	C13H16BFO4
Molecular weight	
Canonicalized Compound	1
Compound Complexity	356
Hydrogen Bond Acceptor Count	5
Hydrogen Bond Donor Count	1
Rotatable Bond Count	2
Allowed IUPAC Name	2-fluoro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoic acid
CAS-like Style IUPAC Name	2-fluoro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoic acid

Specifications	Limits
Markup IUPAC Name	2-fluoro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoic acid
Preferred IUPAC Name	2-fluoro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoic acid
Systematic IUPAC Name	2-fluoranyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoic acid
Traditional IUPAC Name	2-fluoro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoic acid
Standard InChI	InChI=1S/C13H16BFO4/c1-12(2)13(3,4)19-14(18-12)8-5-6-9(11(16)17)10(15)7-8/h5-7H,1-4H3,(H,16,17)
Standard InChIKey	BZWWFDHWZHGLFH-UHFFFAOYSA-N
Exact Mass	266.1125673
Molecular Weight	266.07
Canonical SMILES	B1(OC(C(O1)(C)C)(C)C)C2=CC(=C(C=C2)C(=O)O)F
Chemical Structure	chemicalStructure-4-carboxy-3-fluorobenzeneboronicacid-pinacolester