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Typical Product Specifications & Properties

Benzoic acid, 3-fluoro-4-(formylamino)-, methyl ester

CAS Number: : 1314936-23-6

Specifications	Limits
Chemical Structure	 615611 615611_benzoic-acid-3-fluoro-4-formylamino-methyl-ester.png chemical structure
Chemical Structure	 chemicalStructure-benzoic-acid-3-fluoro-4-formylamino-methyl-ester
Molecular Formula	C9H8FNO3
Molecular weight	
Canonicalized Compound	1
Compound Complexity	222
Hydrogen Bond Acceptor Count	4
Hydrogen Bond Donor Count	1
Rotatable Bond Count	3
Allowed IUPAC Name	methyl 3-fluoro-4-formamido-benzoate
CAS-like Style IUPAC Name	3-fluoro-4-formamidobenzoic acid methyl ester
Markup IUPAC Name	methyl 3-fluoro-4-formamidobenzoate



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Specifications	Limits
Preferred IUPAC Name	methyl 3-fluoro-4-formamidobenzoate
Systematic IUPAC Name	methyl 3-fluoranyl-4-formamido-benzoate
Traditional IUPAC Name	3-fluoro-4-formamido-benzoic acid methyl ester
Standard InChI	InChI=1S/C9H8FNO3/c1-14-9(13)6-2-3-8(11-5-12)7(10)4-6/h2-5H,1H3,(H,11,12)
Standard InChIKey	HECHHBNGQFHWHW-UHFFFAOYSA-N
XLogP3-AA Log P	1.1
Exact Mass	197.04882128
Molecular Weight	197.16
Canonical SMILES	<chem>COC(=O)C1=CC(=C(C=C1)NC=O)F</chem>
Isomeric SMILES	<chem>COC(=O)C1=CC(=C(C=C1)NC=O)F</chem>
Polar Surface Area Topological	55.4
Monoisotopic Weight	197.04882128



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