## 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 |

| 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 | COC(=O)C1=CC(=C(C=C1)NC=O)F |
| Isomeric SMILES | COC(=O)C1=CC(=C(C=C1)NC=O)F |
| Polar Surface Area Topological | 55.4 |
| Monolsotopic Weight | 197.04882128 |