Typical Product Specifications & Properties

1-(5-Bromo-6-fluoropyridin-3-yl)ethanone

CAS Number: : 1256822-63-5

Specifications	Limits
Chemical Structure	615608 615608_1-5-bromo-6-fluoropyridin-3-yl-ethanone.png chemical structure
Chemical Structure	chemicalStructure-1-5-bromo-6-fluoropyridin-3-yl-ethanone
Molecular Formula	C7H5BrFNO
Molecular weight	
Canonicalized Compound	1
Compound Complexity	165
Hydrogen Bond Acceptor Count	3
Hydrogen Bond Donor Count	
Rotatable Bond Count	1
Allowed IUPAC Name	1-(5-bromo-6-fluoro-3-pyridyl)ethanone
CAS-like Style IUPAC Name	1-(5-bromo-6-fluoro-3-pyridinyl)ethanone
Markup IUPAC Name	1-(5-bromo-6-fluoropyridin-3-yl)ethanone

Specifications	Limits
Preferred IUPAC Name	1-(5-bromo-6-fluoropyridin-3-yl)ethanone
Systematic IUPAC Name	1-(5-bromanyl-6-fluoranyl-pyridin-3-yl)ethanone
Traditional IUPAC Name	1-(5-bromo-6-fluoro-3-pyridyl)ethanone
Standard InChI	InChI=1S/C7H5BrFNO/c1-4(11)5-2-6(8)7(9)10-3-5/h2-3H,1H3
Standard InChIKey	MPOPKKNVDNMPBH-UHFFFAOYSA-N
XLogP3-AA Log P	1.7
Exact Mass	216.95385
Molecular Weight	218.02
Canonical SMILES	CC(=O)C1=CC(=C(N=C1)F)Br
Isomeric SMILES	CC(=O)C1=CC(=C(N=C1)F)Br
Polar Surface Area Topological	30
MonoIsotopic Weight	216.95385