Typical Product Specifications & Properties

2-(6-CHLOROPYRIDIN-3-YL)-2-METHYLPROPANENITRILE

CAS Number: : 1095545-86-0

Specifications	Limits
Chemical Structure	
Canonicalized Compound	1
Compound Complexity	204
Hydrogen Bond Acceptor Count	2
Rotatable Bond Count	1
Allowed IUPAC Name	2-(6-chloro-3-pyridyl)-2-methyl-propanenitrile
CAS-like Style IUPAC Name	2-(6-chloro-3-pyridinyl)-2-methylpropanenitrile
Markup IUPAC Name	2-(6-chloropyridin-3-yl)-2-methylpropanenitrile
Preferred IUPAC Name	2-(6-chloropyridin-3-yl)-2-methylpropanenitrile
Systematic IUPAC Name	2-(6-chloranylpyridin-3-yl)-2-methyl-propanenitrile
Traditional IUPAC Name	2-(6-chloro-3-pyridyl)-2-methyl-propionitrile
Standard InChI	InChI=1S/C9H9ClN2/c1-9(2,6-11)7-3-4-8(10)12-5-7/h3-5H,1-2H3

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Specifications	Limits
Standard InChIKey	OLSZBCJEVUIQNV-UHFFFAOYSA-N
XLogP3-AA Log P	2.4
Exact Mass	180.0454260
Molecular Weight	180.63
Canonical SMILES	CC(C)(C#N)C1=CN=C(C=C1)Cl
Isomeric SMILES	CC(C)(C#N)C1=CN=C(C=C1)Cl
Polar Surface Area Topological	36.7
MonoIsotopic Weight	180.0454260

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