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Typical Product Specifications & Properties

5-BROMO-2-(1H-TETRAZOL-5-YL)PYRIDINE

CAS Number: : 380380-60-9

Specifications	Limits
Molecular Formula	C ₆ H ₄ BrN ₅
Molecular weight	
Canonicalized Compound	1
Compound Complexity	155
Hydrogen Bond Acceptor Count	4
Hydrogen Bond Donor Count	1
Rotatable Bond Count	1
Allowed IUPAC Name	5-bromo-2-(2H-tetrazol-5-yl)pyridine
CAS-like Style IUPAC Name	5-bromo-2-(2H-tetrazol-5-yl)pyridine
Markup IUPAC Name	5-bromo-2-(2<I>H</I>-tetrazol-5-yl)pyridine
Preferred IUPAC Name	5-bromo-2-(2H-tetrazol-5-yl)pyridine
Systematic IUPAC Name	5-bromanyl-2-(2H-1,2,3,4-tetrazol-5-yl)pyridine



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Specifications	Limits
Traditional IUPAC Name	5-bromo-2-(2H-tetrazol-5-yl)pyridine
Standard InChI	InChI=1S/C6H4BrN5/c7-4-1-2-5(8-3-4)6-9-11-12-10-6/h1-3H,(H,9,10,11,12)
Standard InChIKey	LBDJSOHAVRCQPD-UHFFFAOYSA-N
XLogP3-AA Log P	0.8
Exact Mass	224.96501
Molecular Weight	226.03
Canonical SMILES	<chem>C1=CC(=NC=C1Br)C2=NNN=N2</chem>
Isomeric SMILES	<chem>C1=CC(=NC=C1Br)C2=NNN=N2</chem>
Polar Surface Area Topological	67.4
Monoisotopic Weight	224.96501
Chemical Structure	 chemicalStructure-5-bromo-2-1h-tetrazol-5-yl-pyridine



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