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Typical Product Specifications & Properties

1H-1,2,4-Triazol-5-amine, 3-(trifluoromethyl)-

CAS Number: : 25979-00-4

Specifications	Limits
Molecular Formula	C3H3F3N4
Molecular weight	
Canonicalized Compound	1
Compound Complexity	123
Hydrogen Bond Acceptor Count	6
Hydrogen Bond Donor Count	2
Rotatable Bond Count	
Allowed IUPAC Name	5-(trifluoromethyl)-1H-1,2,4-triazol-3-amine
CAS-like Style IUPAC Name	5-(trifluoromethyl)-1H-1,2,4-triazol-3-amine
Markup IUPAC Name	5-(trifluoromethyl)-1<H>-1,2,4-triazol-3-amine
Preferred IUPAC Name	5-(trifluoromethyl)-1H-1,2,4-triazol-3-amine
Systematic IUPAC Name	5-(trifluoromethyl)-1H-1,2,4-triazol-3-amine



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Specifications	Limits
Traditional IUPAC Name	[5-(trifluoromethyl)-1H-1,2,4-triazol-3-yl]amine
Standard InChI	InChI=1S/C3H3F3N4/c4-3(5,6)1-8-2(7)10-9-1/h(H3,7,8,9,10)
Standard InChIKey	NQNDVCURMZJFNR-UHFFFAOYSA-N
XLogP3-AA Log P	0.6
Exact Mass	152.03098060
Molecular Weight	152.08
Canonical SMILES	<chem>C1(=NC(=NN1)N)C(F)(F)F</chem>
Isomeric SMILES	<chem>C1(=NC(=NN1)N)C(F)(F)F</chem>
Polar Surface Area Topological	67.6
Monoisotopic Weight	152.03098060
Chemical Structure	 chemicalStructure-1h-1-2-4-triazol-5-amine-3-trifluoromethyl-



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