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Typical Product Specifications & Properties

4-Methyl-2-(4-(trifluoromethyl)phenyl)thiazole-5-carboxylic acid

CAS Number: : 144059-86-9

Specifications	Limits
Chemical Structure	 chemicalStructure-4-methyl-2-(4-trifluoromethyl-phenyl)-thiazole-5-carboxylic-acid
Molecular Formula	C12H8F3NO2S
Molecular weight	
Canonicalized Compound	1
Compound Complexity	342
Hydrogen Bond Acceptor Count	7
Hydrogen Bond Donor Count	1
Rotatable Bond Count	2
Allowed IUPAC Name	4-methyl-2-[4-(trifluoromethyl)phenyl]thiazole-5-carboxylic acid
CAS-like Style IUPAC Name	4-methyl-2-[4-(trifluoromethyl)phenyl]-5-thiazolecarboxylic acid
Markup IUPAC Name	4-methyl-2-[4-(trifluoromethyl)phenyl]-1,3-thiazole-5-carboxylic acid
Preferred IUPAC Name	4-methyl-2-[4-(trifluoromethyl)phenyl]-1,3-thiazole-5-carboxylic acid

ISO 9001

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Specifications	Limits
Systematic IUPAC Name	4-methyl-2-[4-(trifluoromethyl)phenyl]-1,3-thiazole-5-carboxylic acid
Traditional IUPAC Name	4-methyl-2-[4-(trifluoromethyl)phenyl]thiazole-5-carboxylic acid
Standard InChI	InChI=1S/C12H8F3NO2S/c1-6-9(11(17)18)19-10(16-6)7-2-4-8(5-3-7)12(13,14)15/h2-5H,1H3,(H,17,18)
Standard InChIKey	DRFFZMPSUPHSJN-UHFFFAOYSA-N
XLogP3-AA Log P	3.8
Exact Mass	287.02278416
Molecular Weight	287.26
Canonical SMILES	CC1=C(SC(=N1)C2=CC=C(C=C2)C(F)(F)F)C(=O)O
Isomeric SMILES	CC1=C(SC(=N1)C2=CC=C(C=C2)C(F)(F)F)C(=O)O
Polar Surface Area Topological	78.4

Specifications	Limits
Monoisotopic Weight	287.02278416

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