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Typical Product Specifications & Properties

Thieno[3,4-b]-1,4-dioxin-5-carboxylic acid, 2,3-dihydro-

CAS Number: : 260063-21-6

Specifications	Limits
Chemical Structure	 chemicalStructure-thieno-3-4-b-1-4-dioxin-5-carboxylic-acid-2-3-dihydro-
Molecular Formula	C7H6O4S
Molecular weight	
Canonicalized Compound	1
Compound Complexity	196
Hydrogen Bond Acceptor Count	5
Hydrogen Bond Donor Count	1
Rotatable Bond Count	1
Allowed IUPAC Name	2,3-dihydrothieno[3,4-b][1,4]dioxine-5-carboxylic acid
CAS-like Style IUPAC Name	2,3-dihydrothieno[3,4-b][1,4]dioxin-5-carboxylic acid
Markup IUPAC Name	2,3-dihydrothieno[3,4-b][1,4]dioxine-5-carboxylic acid
Preferred IUPAC Name	2,3-dihydrothieno[3,4-b][1,4]dioxine-5-carboxylic acid



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Specifications	Limits
Systematic IUPAC Name	2,3-dihydrothieno[3,4-b][1,4]dioxine-5-carboxylic acid
Traditional IUPAC Name	2,3-dihydrothieno[3,4-b][1,4]dioxin-5-carboxylic acid
Standard InChI	InChI=1S/C7H6O4S/c8-7(9)6-5-4(3-12-6)10-1-2-11-5/h3H,1-2H2,(H,8,9)
Standard InChIKey	DCCRIIFBJZOPAV-UHFFFAOYSA-N
XLogP3-AA Log P	1.2
Exact Mass	185.99867984
Molecular Weight	186.19
Canonical SMILES	<chem>C1COC2=C(SC=C2O1)C(=O)O</chem>
Isomeric SMILES	<chem>C1COC2=C(SC=C2O1)C(=O)O</chem>
Polar Surface Area Topological	84
Monoisotopic Weight	185.99867984



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