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Typical Product Specifications & Properties

2,3-Dimethoxybenzeneboronic acid

CAS Number: : 40972-86-9

Specifications	Limits
Molecular Formula	C8H11BO4
Molecular weight	
Canonicalized Compound	1
Compound Complexity	153
Hydrogen Bond Acceptor Count	4
Hydrogen Bond Donor Count	2
Rotatable Bond Count	3
Allowed IUPAC Name	(2,3-dimethoxyphenyl)boronic acid
CAS-like Style IUPAC Name	(2,3-dimethoxyphenyl)boronic acid
Markup IUPAC Name	(2,3-dimethoxyphenyl)boronic acid
Preferred IUPAC Name	(2,3-dimethoxyphenyl)boronic acid
Systematic IUPAC Name	(2,3-dimethoxyphenyl)boronic acid




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Specifications	Limits
Traditional IUPAC Name	(2,3-dimethoxyphenyl)boronic acid
Standard InChI	InChI=1S/C8H11BO4/c1-12-7-5-3-4-6(9(10)11)8(7)13-2/h3-5,10-11H,1-2H3
Standard InChIKey	VREWSCMOGIXMDQ-UHFFFAOYSA-N
Exact Mass	182.0750390
Molecular Weight	181.98
Canonical SMILES	B(C1=C(C(=CC=C1)OC)OC)(O)O
Isomeric SMILES	B(C1=C(C(=CC=C1)OC)OC)(O)O
Polar Surface Area Topological	58.9
Monoisotopic Weight	182.0750390
Chemical Structure	 chemicalStructure-2-3-dimethoxybenzeneboronic-acid



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