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Typical Product Specifications & Properties

1,2,4-Pyrrolidinetricarboxylic acid, 1-(1,1-dimethylethyl) 2-methyl ester, (2S,4S)-

CAS Number: : 1378388-35-2

Specifications	Limits
Molecular Formula	C12H19NO6
Molecular weight	
Canonicalized Compound	1
Compound Complexity	386
Hydrogen Bond Acceptor Count	6
Hydrogen Bond Donor Count	1
Rotatable Bond Count	5
Allowed IUPAC Name	(3S,5S)-1-tert-butoxycarbonyl-5-methoxycarbonyl-pyrrolidine-3-carboxylic acid
CAS-like Style IUPAC Name	(3S,5S)-5-methoxycarbonyl-1-[(2-methylpropan-2-yl)oxy-oxomethyl]-3-pyrrolidinecarboxylic acid
Markup IUPAC Name	(3<I>S</I>,5<I>S</I>)-5-methoxycarbonyl-1-[(2-methylpropan-2-yl)oxycarbonyl]pyrrolidine-3-carboxylic acid
Preferred IUPAC Name	(3S,5S)-5-methoxycarbonyl-1-[(2-methylpropan-2-yl)oxycarbonyl]pyrrolidine-3-carboxylic acid
Systematic IUPAC Name	(3S,5S)-5-methoxycarbonyl-1-[(2-methylpropan-2-yl)oxycarbonyl]pyrrolidine-3-carboxylic acid

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Specifications	Limits
Traditional IUPAC Name	(3S,5S)-1-tert-butoxycarbonyl-5-carbomethoxy-pyrrolidine-3-carboxylic acid
Standard InChI	InChI=1S/C12H19NO6/c1-12(2,3)19-11(17)13-6-7(9(14)15)5-8(13)10(16)18-4/h7-8H,5-6H2,1-4H3,(H,14,15)/t7-,8-/m0/s1
Standard InChIKey	HMHB AEDPNFIUEI-YUMQZZ PRSA-N
XLogP3-AA Log P	0.7
Exact Mass	273.12123733
Molecular Weight	273.28
Canonical SMILES	CC(C)(C)OC(=O)N1CC(CC1C(=O)OC)C(=O)O
Isomeric SMILES	CC(C)(C)OC(=O)N1C[C@H](C[C@H]1C(=O)OC)C(=O)O
Specifications	Limits

Polar Surface
Area Topological

93.1

Monoisotopic
Weight

273.12123733

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Chemical

Structure



Chemical Structure-1-2-4-pyrrolidinetricarboxylic-acid-1-

1,1-dimethylethyl-2-methyl-ester-2a,4a



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