Typical Product Specifications & Properties

1-Benzylpyrrolidine-3-carbonitrile oxalate

CAS Number: : 1188265-21-5

Specifications	Limits
Chemical Structure	chemicalStructure-1-benzylpyrrolidine-3-carbonitrile-oxalate
Molecular Formula	C14H16N2O4
Molecular weight	
Canonicalized Compound	1
Compound Complexity	293
Hydrogen Bond Acceptor Count	6
Hydrogen Bond Donor Count	2
Rotatable Bond Count	3
Allowed IUPAC Name	1-benzylpyrrolidine-3-carbonitrile;oxalic acid
CAS-like Style IUPAC Name	oxalic acid;1-(phenylmethyl)-3-pyrrolidinecarbonitrile
Markup IUPAC Name	1-benzylpyrrolidine-3-carbonitrile;oxalic acid
Preferred IUPAC Name	1-benzylpyrrolidine-3-carbonitrile;oxalic acid

Specifications	Limits
Systematic IUPAC Name	ethanedioic acid;1-(phenylmethyl)pyrrolidine-3-carbonitrile
Traditional IUPAC Name	1-benzylpyrrolidine-3-carbonitrile;oxalic acid
Standard InChI	InChI=1S/C12H14N2.C2H2O4/c13-8-12-6-7-14(10-12)9-11-4-2-1-3-5-11;3-1(4)2(5)6/h1-5,12H,6-7,9-10H2;(H,3,4)(H,5,6)
Standard InChIKey	NLBJMBNDZZMLDI-UHFFFAOYSA-N
Exact Mass	276.11100700
Molecular Weight	276.29
Canonical SMILES	C1CN(CC1C#N)CC2=CC=CC=C2.C(=O)(C(=O)O)O
Isomeric SMILES	C1CN(CC1C#N)CC2=CC=CC=C2.C(=O)(C(=O)O)O
Polar Surface Area Topological	102
Monolsotopic Weight	276.11100700