Typical Product Specifications & Properties

Carbamic acid, N-(1,2-dihydro-2-oxo-4-pyridinyl)-, 1,1-dimethylethyl ester

CAS Number: : 1363383-37-2

Specifications	Limits
Chemical Structure	615605 615605_carbamic-acid-n-1-2-dihydro-2-oxo-4-pyridinyl-1-1-dimethylethyl-ester.png chemical structure
Molecular Formula	C10H14N2O3
Molecular weight	
Canonicalized Compound	1
Compound Complexity	337
Hydrogen Bond Acceptor Count	3
Hydrogen Bond Donor Count	2
Rotatable Bond Count	3
Allowed IUPAC Name	tert-butyl N-(2-oxo-1H-pyridin-4-yl)carbamate
CAS-like Style IUPAC Name	N-(2-oxo-1H-pyridin-4-yl)carbamic acid tert-butyl ester
Markup IUPAC Name	<I>tert</I>-butyl <I>N</I>-(2-oxo-1<I>H</I>-pyridin-4-yl)carbamate
Preferred IUPAC Name	tert-butyl N-(2-oxo-1H-pyridin-4-yl)carbamate

Specifications	Limits
Systematic IUPAC Name	tert-butyl N-(2-oxidanylidene-1H-pyridin-4-yl)carbamate
Traditional IUPAC Name	N-(2-keto-1H-pyridin-4-yl)carbamic acid tert-butyl ester
Standard InChI	InChI=1S/C10H14N2O3/c1-10(2,3)15-9(14)12-7-4-5-11-8(13)6-7/h4-6H,1-3H3,(H2,11,12,13,14)
Chemical Structure	 chemicalStructure-carbamic-acid-n-1-2-dihydro-2-oxo-4-pyridinyl-1-1-dimethylethyl-ester
Standard InChIKey	VNJZRTVKUGFQOP-UHFFFAOYSA-N
XLogP3-AA Log P	0.5
Exact Mass	210.10044231
Molecular Weight	210.23
Canonical SMILES	CC(C)(C)OC(=O)NC1=CC(=O)NC=C1
Isomeric SMILES	CC(C)(C)OC(=O)NC1=CC(=O)NC=C1

Specifications	Limits
Polar Surface Area	67.4
Topological Monoisotopic Weight	210.10044231