Typical Product Specifications & Properties

3-Amino-6-Aza-Bicyclo[3.2.1]Octane-6-Carboxylic Acid Tert-Butyl Ester

CAS Number: : 1199942-73-8

Specifications	Limits
Molecular Formula	C12H22N2O2
Molecular weight	
Canonicalized Compound	1
Compound Complexity	285
Hydrogen Bond Acceptor Count	3
Hydrogen Bond Donor Count	1
Rotatable Bond Count	2
Allowed IUPAC Name	tert-butyl 3-amino-6-azabicyclo[3.2.1]octane-6-carboxylate
CAS-like Style IUPAC Name	3-amino-6-azabicyclo[3.2.1]octane-6-carboxylic acid tert-butyl ester
Markup IUPAC Name	<I>tert</I>-butyl 3-amino-6-azabicyclo[3.2.1]octane-6-carboxylate
Preferred IUPAC Name	tert-butyl 3-amino-6-azabicyclo[3.2.1]octane-6-carboxylate
Systematic IUPAC Name	tert-butyl 3-azanyl-6-azabicyclo[3.2.1]octane-6-carboxylate

Specifications	Limits
Traditional IUPAC Name	3-amino-6-azabicyclo[3.2.1]octane-6-carboxylic acid tert-butyl ester
Standard InChI	InChI=1S/C12H22N2O2/c1-12(2,3)16-11(15)14-7-8-4-9(13)6-10(14)5-8/h8-10H,4-7,13H2,1-3H3
Standard InChIKey	NJWVSZHCSYPIMS-UHFFFAOYSA-N
XLogP3-AA Log P	1.2
Exact Mass	226.168127949
Molecular Weight	226.32
Canonical SMILES	CC(C)(C)OC(=O)N1CC2CC(CC1C2)N
Isomeric SMILES	CC(C)(C)OC(=O)N1CC2CC(CC1C2)N
Polar Surface Area Topological	55.6
MonoIsotopic Weight	226.168127949

Specifications	Limits
Chemical Structure	 chemicalStructure-3-amino-6-aza-bicyclo-3.2.1-octane-6-carboxylic-acid-tert-butyl-ester