Typical Product Specifications & Properties

N,N-Dimethyloctanamide

CAS Number: : 1118-92-9

Specifications	Limits
Chemical Structure	chemicalStructure-l-proline-1-o-1-1-dimethylethyl-n-9h-fluoren-9-ylmethoxy-carbonyl-l-seryl-
Molecular Formula	C27H32N2O6
Molecular weight	
Canonicalized Compound	1
Compound Complexity	758
Hydrogen Bond Acceptor Count	6
Hydrogen Bond Donor Count	2
Rotatable Bond Count	9
Allowed IUPAC Name	(2S)-1-[(2S)-3-tert-butoxy-2-(9H-fluoren-9-ylmethoxycarbonylamino)propanoyl]pyrrolidine-2-carboxylic acid
CAS-like Style IUPAC Name	(2S)-1-[(2S)-2-[[9H-fluoren-9-ylmethoxy(oxo)methyl]amino]-3-[(2-methylpropan-2-yl)oxy]-1-oxopropyl]-2-pyrrolidinecarboxylic acid
Markup IUPAC Name	(2<I>S</I>)-1-[(2<I>S</I>)-2-(9<I>H</I>-fluoren-9-ylmethoxycarbonylamino)-3-[(2-methylpropan-2-yl)oxy]propanoyl]pyrrolidine-2-carboxylic acid
Preferred IUPAC Name	(2S)-1-[(2S)-2-(9H-fluoren-9-ylmethoxycarbonylamino)-3-[(2-methylpropan-2-yl)oxy]propanoyl]pyrrolidine-2-carboxylic acid

Specifications	Limits
Systematic IUPAC Name	(2S)-1-[(2S)-2-(9H-fluoren-9-ylmethoxycarbonylamino)-3-[(2-met yl)oxy]propanoyl]pyrrolidine-2-carboxylic acid
Traditional IUPAC Name	(2S)-1-[(2S)-3-tert-butoxy-2-(9H-fluoren-9-ylmethoxycarbonylamino)propanoyl]proline
Standard InChI	InChI=1S/C27H32N2O6/c1-27(2,3)35-16-22(24(30)29-14-8-13-23 26(33)34-15-21-19-11-6-4-9-17(19)18-10-5-7-12-20(18)21/h4-7,9-1 16H2,1-3H3,(H,28,33)(H,31,32)/t22-,23-/m0/s1
Standard InChIKey	ZEGKALAMRJSQJC-GOTSBHOMSA-N
XLogP3-AA Log P	3.6
Exact Mass	480.22603674
Molecular Weight	480.6

Specifications	Limits

Canonical SMILES	CC(C)(C)OC(C(=O)N1CCCC1C(=O)O)NC(=O)OCC2C3=CC=CC=
Isomeric SMILES	CC(C)(C)OC[C@@H](C(=O)N1CCC[C@H]1C(=O)O)NC(=O)OCC2C3=CC=CC=C3C
Polar Surface Area	105

Aled Topological	105
Monolsotopic Weight	480.22603674