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Typical Product Specifications & Properties

(S)-5-(amidinoamino)-2-(benzoylamino)-N-(4-nitrophenyl)valeramide monohydrochloride

CAS Number: : 21653-40-7

Specifications	Limits
Molecular weight	434.88
EINECS	244-505-6
SMILES	<chem>c1ccc(cc1)C(=O)N[C@@H](CCCNC(=N)N)C(=O)Nc2ccc(cc2)[N+](=O)[O-].[Cl-]</chem>
InChI	DEOKFPFLXFNAON-NTISSMGPSA-N
InChIKey	1S/C19H22N6O4.ClH/c20-19(21)22-12-4-7-16(24-17(26)13-5-2-1-3-6-13)18(27)23-14-8-10-15(11-9-14)25(28)29;/h1-3,5-6,8-11,16H,4,7,12H2,(H,23,27)(H,24,26)(H4,20,21,22);1H/t16-/m0./s1
Storage Temperature	-20°C
Color	White to Yellow
Solubility	Soluble in DMSO at 50mg/ml
Melting Point	223-226 °C
Form	Powder



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