

Typical Product Specifications & Properties

TOCINOICACID

CAS Number: : 34330-23-9

Specifications	Limits
Molecular weight	740.86
SMILES	<chem>CC[C@H](C)C1C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N1)Cc2ccc(cc2)O)N)C(=O)O)CC(=O)N)CCC(=O)N</chem>
InChI	ITRWUGOBSKHPTA-LYZHYIKWSA-N
InChIKey	1S/C30H44N8O10S2/c1-3-14(2)24-29(46)34-18(8-9-22(32)40)26(43)36-20(11-23(33)41)27(44)37-21(30(47)48)13-50-49-12-17(31)25(42)35-19(28(45)38-24)10-15-4-6-16(39)7-5-15/h4-7,14,17-21,24,39H,3,8-13,31H2,1-2H3,(H2,32,40)(H2,33,41)(H,34,46)(H,35,42)(H,36,43)