

Typical Product Specifications & Properties

Sulbutiamine

CAS Number: : 3286-46-2

Specifications Limits

Molecular weight	702.89
EINECS	221-937-3
SMILES	<chem>Cc1ncc(CN(C=O)C(\C)=C(/SSC(\CCOC(C(C)C)=O)=C(\C)N(C=O)Cc2cnc(C)nc2N)CCOC(C(C)C)=O)c(N)n1</chem>
InChI	CKHJPWQVLKHBIH-GPAWKIAZSA-N
InChIKey	1S/C32H46N8O6S2/c1-19(2)31(43)45-11-9-27(21(5)39(17-41)15-25-13-35-23(7)37-29(25)33)47-48-28(10-12-46-32(44)20(3)4)22(6)40(18-42)16-26-14-36-24(8)38-30(26)34/h13-14,17-20H,9-12,15-16H2,1-8H3,(H2,33,35,37)(H2,34,36,38)/b27-21+,28-22+