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Typical Product Specifications & Properties

2-[2-[[5,6-dimethyl-3-[3-(sulphonatooxy)propyl]-3H-benzothiazol-2-ylidene]methyl]-1-butenyl]-1-ethyl

CAS Number: : 83721-33-9

Specifications	Limits
Molecular weight	580.78
EINECS	280-562-3
SMILES	<chem>CC/C(=C/c1[n+](c2c3ccccc3ccc2s1)CC)/C=C\4/N(c5cc(c(cc5S4)C)C)CCC(=O)[O-]</chem>
InChI	YPAKGQWVNWDBAZ-UHFFFAOYSA-N
InChIKey	1S/C30H32N2O4S3/c1-5-22(18-28-31(6-2)30-24-11-8-7-10-23(24)26(30)37-28)19-29-32(14-9-15-36-39(33,34)35)25-16-20(3)21(4)127(25)38-29/h7-8,10-13,16-19H,5-6,9,14-15H2,1-4H3



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