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Typical Product Specifications & Properties

(+)-[2-[4-(benzoyloxy)-3-(methylthio)phenyl]-2-oxoethyl][3-(4-methoxyphenyl)-1-methylpropyl]ammonium

CAS Number: : 66264-97-9

Specifications	Limits
Molecular weight	544.50
EINECS	266-292-9
SMILES	<chem>CC(CCCc1ccc(cc1)OC)[NH2+]CC(=O)c2ccc(c(c2)SC)OC(=O)c3ccccc3.[Br-]</chem>
InChI	ARYLHJDBGBQPIV-UHFFFAOYSA-N
InChIKey	1S/C27H29NO4S.BrH/c1-19(9-10-20-11-14-23(31-2)15-12-20)28-18-24(29)22-13-16-25(26(17-22)33-3)32-27(30)21-7-5-4-6-8-21;/h4-8,11-17,19,28H,9-10,18H2,1-3H3;1H



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