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Typical Product Specifications & Properties

Calmidazolium

CAS Number: : 95013-41-5

Specifications	Limits
SMILES	<chem>c1[n+](ccn1C(c1ccc(cc1)Cl)c1ccc(cc1)Cl)C[C@@H](OCc1c(cc(cc1)Cl)Cl)c1c(cc(cc1)Cl)Cl</chem>
InChI	CTKNMSVWMRRCPW-UHFFFAOYSA-N
InChIKey	1S/C31H23Cl6N2O/c32-23-6-1-20(2-7-23)31(21-3-8-24(33)9-4-21)39-14-13-38(19-39)17-30(27-12-11-26(35)16-29(27)37)40-18-22-5-10-25(34)15-28(22)36/h1-16,19,30-31H,17-18H2/q+1



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