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Typical Product Specifications & Properties

CALMAGITE TRIETHANOLAMMONIUM

CAS Number: : 91698-30-5

Specifications	Limits
Molecular weight	459.56
SMILES	<chem>N(CCO)(CCO)CCO.c1(cc(c(c2ccccc12)\N=N\c1c(ccc(c1)C)O)O)S(=O)O</chem>
InChI	NOCQPFRKSJKVKW-LTRPLHCISA-N
InChIKey	1S/C17H14N2O5S.C6H15NO3/c1-10-6-7-14(20)13(8-10)18-19-17-5-3-2-4-11(12)16(9-15(17)21)25(22,23)24;8-4-1-7(2-5-9)3-6-10/h2,9,20-21H,1H3,(H,22,23,24);8-10H,1-6H2/b19-18+;



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