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Typical Product Specifications & Properties

Acid blue 3

CAS Number: : 3536-49-0

Specifications	Limits
Molecular weight	1,159.44
SMILES	<chem>C1(\C=C\C(=[N+](\CC)CC)C=C1)=C(/c1ccc(N(CC)CC)cc1)c1c(S(=O)(=O)[O-])cc(c(c1)O)S(=O)(=O)[O-].[Ca+2].C1(=C(/c2ccc(N(CC)CC)cc2)c2cc(O)c(S(=O)(=O)[O-])cc2S(=O)(=O)[O-])\C=C\C(=[N+](\CC)CC)C=C1</chem>
InChI	RTMBGDDBDQKNNZ-UHFFFAOYSA-L
InChIKey	1S/2C27H32N2O7S2.Ca/c2*1-5-28(6-2)21-13-9-19(10-14-21)27(20-11-15-22(16-12-20)29(7-3)8-4)23-17-24(30)26(38(34,35)36)18-25(23)37(31,32)33;/h2*9-18H,5-8H2,1-4H3,(H2-,30,31,32,33,34,35,36);/q;+2/p-2

