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Typical Product Specifications & Properties

1H-Pyrazole-3-carboxylic acid, 5-hydroxy-4-[[5-[[4-[5-hydroxy-3-methyl-4-[[2-sulfo-5-(2,5,6-trichlo

CAS Number: : 70210-12-7

Specifications	Limits
Molecular weight	1,152.15
EINECS	274-408-4
SMILES	<chem>[Na+].[Na+].[Na+].[Na+].N1(N=C([C@@H](C1=O)\N=N\c1c(ccc(c1)NC(c1ccc(cc1)N1N=C([C@@H](C1=O)\N=N\c1c(ccc(c1)Nc1nc(nc(c1Cl)Cl)Cl)S(=O)(=O)[O-])C=O)S(=O)(=O)[O-])C(=O)[O-])c1ccc(cc1)S(=O)(=O)[O-]</chem>
InChI	XIXZXVKCIZGDOM-JMYUTWMGSA-J
InChIKey	1S/C37H25Cl3N12O14S3.4Na/c1-16-28(47-45-23-14-18(4-12-25(23)68(61,62)63)41-32-27(38)31(39)43-37(40)44-32)34(54)51(49-16)20-6-2-17(3-7-20)33(53)42-19-5-13-26(69(64,65)66)24(15-19)46-48-29-30(36(56)57)50-52(35(29)55)21-8-10-22(11-9-21)67(58,59)60;;;/h



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