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Typical Product Specifications & Properties

2-amino-5-[[2-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]-2-sulphophenyl]azo]-3-oxobutyroyl]ami

CAS Number: : 83399-90-0

Specifications	Limits
Molecular weight	765.97
EINECS	280-403-8
SMILES	<chem>CC(=O)C(C(=O)Nc1cc(c(c(c1)S(=O)(=O)[O-])N)S(=O)(=O)[O-])/N=N/c2ccc(cc2S(=O)(=O)[O-])Nc3c(c(nc(n3)F)F)Cl.[Na+].[Na+].[Na+]</chem>
InChI	RCZVWBMNZFKWOD-MHAWFHQYSA-K
InChIKey	1S/C20H16ClF2N7O11S3.3Na/c1-7(31)16(19(32)26-9-5-12(43(36,37)38)15(24)13(6-9)44(39,40)41)30-29-10-3-2-8(4-11(10)42(33,34)35)25-18-14(21)17(22)27-20(23)28-18;;;/h2-6,16H,24H2,1H3,(H,26,32)(H,25,27,28)(H,33,34,35)(H,36,37,38)(H,39,40,41);;;/q:3*+1/p-3/



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