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Typical Product Specifications & Properties

2-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]-6-[[4,5-dihydro-3-methyl-5-oxo-1-(4-sulphophenyl)-1H-

CAS Number: : 83400-22-0

Specifications	Limits
Molecular weight	659.94
EINECS	280-438-9
SMILES	<chem>Cc1c(cc(cc1/N=N/C2C(=NN(C2=O)c3ccc(cc3)S(=O)(=O)[O-])C)S(=O)(=O)[O-])Nc4c(c(nc(n4)F)F)Cl.[Na+].[Na+]</chem>
InChI	IJCMZANLDDGSKI-NTDCDQ.SISA-L
InChIKey	1S/C21H16ClF2N7O7S2.2Na/c1-9-14(25-19-16(22)18(23)26-21(24)27-19)7-13(40(36,37)38)8-15(9)28-29-17-10(2)30-31(20(17)32)11-3-5-12(6-4-11)39(33,34)35;;/h3-8,17H,1-2H3,(H,25,26,27)(H,33,34,35)(H,36,37,38);;/q;2*+1/p-2/b29-28+;;



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