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Typical Product Specifications & Properties

2-[2-[2,3-dihydro-5-methyl-3-oxo-2-phenyl-1-(4-sulphonatobutyl)-1H-pyrazol-4-yl]-3-(6-methoxy-3-meth

CAS Number: : 2321-65-5

Specifications	Limits
Molecular weight	704.88
EINECS	219-032-3
SMILES	<chem>c1(c(n(c2ccccc2)n(c1C)CCCCS(=O)(=O)[O-])=O)C(\C=C1\N(c2ccc(cc2S1)OC)C)=C/c1[n+](c2ccc(cc2s1)OC)C</chem>
InChI	WVXXUIKUBNLFPA-UHFFFAOYSA-N
InChIKey	1S/C35H36N4O6S3/c1-23-34(35(40)39(25-11-7-6-8-12-25)38(23)17-9-10-18-48(41,42)43)24(19-32-36(2)28-15-13-26(44-4)21-30(28)46-32)20-33-37(3)29-16-14-27(45-5)22-31(29)47-33/h6-8,11-16,19-22H,9-10,17-18H2,1-5H3



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