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Typical Product Specifications & Properties

2-[[5-[4-(methoxycarbonyl)phenyl]-3-methyl-1,3,4-thiadiazol-2(3H)-ylidene]methyl]-1-methylquinolinium

CAS Number: : 85050-06-2

Specifications	Limits
Molecular weight	501.58
EINECS	285-278-3
SMILES	<chem>C[n+](c(ccc2c1cccc2)/C=C\3/N(N=C(S3)c4ccc(cc4)C(=O);(=O)[O-]</chem>
InChI	MGBJLQOGUZXASV-UHFFFAOYSA-M
InChIKey	1S/C22H20N3O2S.CH4O4S/c1-24-18(13-12-15-6-4-5-7-19(15)24)21(28-20)16-8-10-17(11-9-16)22(26)27-3;1-5-6(2,3)4/h4-14H,1-3H(H,2,3,4)/q+1;/p-1



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