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Typical Product Specifications & Properties

1-(8-chloro-10,11-dihydrodibenzo[b,f]thiepin-10-yl)-4-methylpiperazinium methanesulphonate

CAS Number: : 42505-79-3

Specifications	Limits
Molecular weight	441.01
EINECS	255-855-4
SMILES	<chem>N1([C@@H]2Cc3c(Sc4c2cc(cc4)Cl)cccc3)CCN(C)CC1.CS(=O)(=O)O</chem>
InChI	XQRUOHZMMIUQSB-UHFFFAOYSA-N
InChIKey	1S/C19H21ClN2S.CH4O3S/c1-21-8-10-22(11-9-21)17-12-14-4-2-3-5-18(14)23-19-7-6-15(20)13-16(17)19;1-5(2,3)4/h2-7,13,17H,8-12H2,1H3;1H3,(H,2,3,4)



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