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Typical Product Specifications & Properties

Sodium Hydrogen -5-[(1,2-Dimethyl-1H-Indol-3-yl)[4-[(O-Tolyl)Imino]-3-Sulphonato-2,5-Cyclohexadien-1

CAS Number: : 94275-71-5

Specifications	Limits
Molecular weight	701.79
EINECS	304-459-0
SMILES	<chem>Cc1ccccc1Nc2ccc(cc2S(=O)(=O)O)/C(=C/3\C=C/C(=N\c4ccccc4C)/C(=C3)S(=O)(=O)[O-])/c5c(n(c6c5ccccc6)C)C.[Na+]</chem>
InChI	HEWMUQJYCTVCCB-IUOVKKGRSA-M
InChIKey	1S/C37H33N3O6S2.Na/c1-23-11-5-8-14-29(23)38-31-19-17-26(21-34(31)47(41,42)43)37(36-25(3)40(4)33-16-10-7-13-28(33)36)27-18-20-32(35(22-27)48(44,45)46)39-30-15-9-6-12-24(30)2;/h5-22,38H,1-4H3,(H,41,42,43)(H,44,45,46);/q;+1/p-1/b37-27-,39-32+;



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