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Typical Product Specifications & Properties

Octhilinone

CAS Number: : 26530-20-1

Specifications	Limits
Molecular weight	213.34
EINECS	247-761-7
InChI	1S/C11H19NOS/c1-2-3-4-5-6-7-9-12-11(13)8-10-14-12/h8,10H,2-7,9H2,1H3
InChIKey	JPMIIZHYYYWMHDT-UHFFFAOYSA-N
Stability	Stable. Incompatible with strong oxidizin
Density	1.04
Boiling Point	120°C
Storage Temperature	Refrigerator
Water solubility	<0.1 g/100 mL at 19 ºC
Molecular weight	590.49
EINECS	239-201-5
SMILES	c12c(c(ccc1/N=N\c1c(nn(c1O)c1ccc(cc1)S(=O)(=O)[O-])C(=O)OCC)S(=O)(=O)[O-])cccc2.[Na+].[Na+]



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Specifications	Limits
InChI	BLQVZCMYWIKAGV-KPOOZVEVSA-L
InChIKey	1S/C22H18N4O9S2.2Na/c1-2-35-22(28)20-19(21(27)26(25-20)13-7-9-14(10-8-13)36(29,30)31)24-23-17-11-12-18(37(32,33)34)16-6-4-3-5-15(16)17;/h3-12,19H,2H2,1H3,(H,29,30,31)(H,32,33,34)/;:/q;2*+1/p-2/b24-23+;;



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