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Typical Product Specifications & Properties

CI 16035

CAS Number: : 25956-17-6

Specifications	Limits
Molecular weight	496.43
SMILES	<chem>c12c(cc(cc2)S(=O)(=O)[O-])ccc(c1/N=N/c1c(cc(c(c1)C)S(=O)(=O)[O-])OC)O.[Na+].[Na+]</chem>
InChI	CEZ CCHQBSQPRMU-LLIZZ RELSA-L
InChIKey	1S/C18H16N2O8S2.2Na/c1-10-7-14(16(28-2)9-17(10)30(25,26)27)19-20-18-13-5-4-12(29(22,23)24)8-11(13)3-6-15(18)21;;/h3-9,21H,1-2H3,(H,22,23,24)(H,25,26,27);;/q;2*+1/p-2/b20-19+;;
Water solubility	2.25E+05 mg/L
Atmospheric OH Rate Constant	7.05E-12 cm ³ /molecule-sec
log P (octanol-water)	-0.550



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