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Typical Product Specifications & Properties

Brown HT

CAS Number: : 4553-89-3

Specifications	Limits
Molecular weight	652.56
EINECS	224-924-0
SMILES	<chem>c12c(c(\N=N\c3c(c(\N=N\c4c5c(c(S(=O)(=O)[O-])cc4)cccc5)cc(c3O)CO)O)ccc1S(=O)(=O)[O-])cccc2.[Na+].[Na+]</chem>
InChI	BIRIBMFCDVVRKL-DBHLKOEUSA-L
InChIKey	1S/C27H20N4O9S2.2Na/c32-14-15-13-22(30-28-20-9-11-23(41(35,36)37)18-7-3-1-5-16(18)20)27(34)25(26(15)33)31-29-21-10-12-24(42(38,39)40)19-8-4-2-6-17(19)21;;/h1-13,32-34H,14H2,(H,35,36,37)(H,38,39,40);;/q;2*+1/p-2/b30-28+,31-29+;;



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