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Typical Product Specifications & Properties

Brilliant Blue R soln.

CAS Number: : 6104-59-2

Specifications	Limits
Molecular weight	825.97
EINECS	228-060-5
SMILES	<chem>C(\c1ccc(N(Cc2cc(ccc2)S(=O)(=O)[O-])CC)cc1)(=C1/C=C\C(=[N+](\Cc2cc(ccc2)S(=O)(=O)[O-])CC)C=C1)c1ccc(Nc2ccc(OCC)cc2)cc1.[Na+]</chem>
InChI	NKLPQNGYXWVELD-UHFFFAOYSA-M
InChIKey	1S/C45H45N3O7S2.Na/c1-4-47(31-33-9-7-11-43(29-33)56(49,50)51)40-23-15-36(16-24-40)45(35-13-19-38(20-14-35)46-39-21-27-42(28-22-39)55-6-3)37-17-25-41(26-18-37)48(5-2)32-34-10-8-12-44(30-34)57(52,53)54;/h7-30H,4-6,31-32H2,1-3H3,(H2,49,50,51,52,53,54);/q
Storage Temperature	Store at room temperature.
Colour Index	42660
Water solubility	Soluble in water.
Flash Point	14 °C
Melting Point	174-180 °C



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