

# Product Data Sheet

## (2N) 99% Bromothymol Blue Sodium Salt Solution

Product Code: NA-OMX-02

**Formula:** C<sub>27</sub>H<sub>27</sub>Br<sub>2</sub>O<sub>5</sub>SNa

**CAS No.:** 34722-90-2

**EC No.:** 252-169-7

**MDL:** MFCD00077263

### Chemical Identifiers

|                         |   |
|-------------------------|---|
| <b>Linear Formula</b>   | C <sub>27</sub> H <sub>27</sub> Br <sub>2</sub> O <sub>5</sub> SNa  |
| <b>MDL Number</b>       | MFCD00077263  |
| <b>EC No.</b>           | 252-169-7   |
| <b>Pubchem CID</b>      | 5157491   |
| <b>IUPAC Name</b>       | sodium; 2-[(E)-(3-bromo-4-hydroxy-2-methyl-5-propan-2-ylphenyl)-(3-bromo-2-methyl-4-oxo-5-propan-2-ylcyclohexa-2,5-dien-1-ylidene)methyl]benzenesulfonate                           |
| <b>SMILES</b>           | CC1=C(C=C(C=C1C(=C2C=C(C(=O)C(=C2C)Br)C(C)C)C3=CC=CC=C3S(=O)(=O)[O-])C(C)C)O)Br.[Na+]   |
| <b>Inchi Identifier</b> | InChI=1S/C27H28Br2O5S.Na/c1-13(2)18-11-20(15(5)24(28)26(18)30)23(17-9-7-8-10-22(17)35(32,33)34)21-12-19(14(3)4)27(31)25(29)16(21)6;/h7-14,30H,1-6H3,(H,32,33,34);/q;+1/p-1/b23-21-; |
| <b>Inchi Key</b>        | NMKFVGALBGZKGW-VZXGSGAOSA-M   |

**Total Metal Impurities:** 1.0% max.

### Packaging Specifications

Typical bulk packaging includes palletized plastic 5 gallon/25 kg. pails, fiber and steel drums to 1 ton super sacks in full container (FCL) or truck load (T/L) quantities. Research and sample quantities and hygroscopic, oxidizing or other air sensitive materials may be packaged under argon or vacuum. Shipping documentation includes a Certificate of Analysis and Safety Data Sheet (SDS). Solutions are packaged in polypropylene, plastic or glass jars up to palletized 440 gallon liquid totes, and 36,000 lb. tanker trucks.

#### Documentation

A Certificate of Analysis and Materials Safety Data Sheet (SDS) in accordance with EN 10204 are supplied with every shipment.