

**Product Name:** Thiotriazinone, 98+%, Thermo Scientific Chemicals  
**Catalog Number:** B22663.09

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**CAS Number:** 58909-39-0  
**IUPAC Name:** 2-methyl-3-sulfanylidene-1,2,4-triazinane-5,6-dione  
**Molecular Formula:** C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub>S  
**Molecular Weight:** 159.16  
**InChI Key:** UMWWHOXOVPIGFD-UHFFFAOYSA-N  
**SMILES:** CN1NC(=O)C(=O)NC1=S  
**Synonym:** 2-methyl-3-sulfanylidene-1,2,4-triazinane-5,6-dione

### Product Specification

**Appearance (Color):** White  
**Form:** Powder  
**Assay from Supplier's CofA:** ≥98.0%  
**Water Content (Karl Fischer Titration):** ≤1.0%  
**Melting Point (clear melt):** 247.5-253.5°C  
**Sulfated Ash:** ≤1.0%

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**Date Of Print:** 05/29/2025

*Product Specifications are subject to amendment and may change over time. Data contained is accurate as of the date printed.*