

**Catalog Number:** J65111.06

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**CAS Number:** 5878-61-5  
**IUPAC Name:** 7-(2-chloroethyl)-1,3-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione  
**Molecular Formula:** C<sub>9</sub>H<sub>11</sub>ClN<sub>4</sub>O<sub>2</sub>  
**Molecular Weight:** 242.66  
**InChI Key:** QCIARNIKNKKHFH-UHFFFAOYSA-N  
**SMILES:** CN1C2=C(N(CCCI)C=N2)C(=O)N(C)C1=O  
**Synonym:** 7-(2-chloroethyl)theophylline

### Product Specification

**Appearance (Color):** White  
**Form:** Powder  
**Assay (unspecified):** 97.0% min.

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**Date Of Print:** 04/23/2025

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