

**Product Name:** 4-Nitrophenyl isocyanate, 97%, Thermo Scientific Chemicals  
**Catalog Number:** A11194.06

---

**CAS Number:** 100-28-7  
**IUPAC Name:** 1-isocyanato-4-nitrobenzene  
**Molecular Formula:** C<sub>7</sub>H<sub>4</sub>N<sub>2</sub>O<sub>3</sub>  
**Molecular Weight:** 164.12  
**InChI Key:** GFNKTLQTQSALEJ-UHFFFAOYSA-N  
**SMILES:** [O-][N+](=O)C1=CC=C(C=C1)N=C=O  
**Synonym:** benzene, 1-isocyanato-4-nitro-

### Product Specification

**Appearance (Color):** Yellow  
**Form:** Crystals or powder or crystalline powder or fused solid  
**Melting Point (clear melt):** 53.0-62.0°C  
**Assay (GC):** ≥96.0%  
**Identification (FTIR):** Conforms

---

**Date Of Print:** 12/25/2024

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