

**Product Name:** N-Boc-L-isoleucine, 98+%  
**Catalog Number:** A16021.14

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**CAS Number:** 13139-16-7  
**IUPAC Name:** (2S,3S)-2-[[tert-butoxy)carbonyl]amino]-3-methylpentanoic acid  
**Molecular Formula:** C<sub>11</sub>H<sub>21</sub>NO<sub>4</sub>  
**Molecular Weight:** 231.29  
**MDL Number:** MFCD00038324 MFCD00237550  
**InChI Key:** QJCNLJWUIOIMMF-YUMQZZPRSA-N  
**SMILES:** CC[C@H](C)[C@H](NC(=O)OC(C)(C)C)C(O)=O  
**Synonym:** (2S,3S)-2-[(tert-butoxycarbonyl)amino]-3-methylpentanoic acid

### Product Specification

**Appearance (Color):** White to pale cream  
**Form:** Powder or crystalline powder or crystals or lumps  
**Assay (Aqueous acid-base Titration):** ≥98.0 to ≤102.0% (non-U.S. specification)  
**Assay (HPLC):** ≥98.0% (U.S. specification)  
**Comment:** Specification differs for U.S. and non-U.S. material where indicated  
**Identification (FTIR):** Conforms (U.S. specification)  
**Melting point:** 69-73°C (U.S. specification)  
**Proton NMR:** Conform to structure (U.S. specification)  
**Optical Rotation:** +2.5° to +2.9° (c=2, Acetic acid)  
**Solubility:** Clear solution (0.3g in 2ml of water) (U.S. specification)

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**Date Of Print:** 05/09/2026

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