

Product Name: N-Boc-L-isoleucine, 98+%

Catalog Number: A16021.14

CAS Number: 13139-16-7

IUPAC Name: (2S,3S)-2-[[tert-butoxy)carbonyl]amino]-3-methylpentanoic acid

Molecular Formula: C₁₁H₂₁NO₄

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)

Date Of Print: 01/01/2026

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