

MATERIAL SAFETY DATA SHEET

Section 1 - Identification	
Product identifier	DOTA-tris(tBu ester)
Catalog No.	AS2119
Other identifiers	DOTA-tris(t-butyl ester); tri-tert-butyl protected DOTA with one free acetate carboxyl
Recommended use	Laboratory research, chemical synthesis and peptide-building-block applications.
Restrictions on use	For research use only. Not for human or veterinary use, therapeutic use, diagnostic use, food, household, or consumer applications.
Responsible party	Alan Scientific Inc.
U.S. address	9031 Shady Grove Court, Gaithersburg, MD 20877 U.S.
Contact	+1 888-757-1116 contactus@alanscientific.com www.alanscientific.com
Emergency telephone	+1 888-757-1116

Section 2 - Hazard(s) Identification	
OSHA HCS classification	No specific GHS hazard classification assigned in this document based on the public supplier information reviewed. Toxicological data may be incomplete.
Signal word	None assigned
Hazard statements	None assigned in this document.
Pictograms	None assigned
Precautionary statements	Handle as a laboratory research chemical. Avoid breathing dust and unnecessary skin or eye contact. Wear suitable gloves and eye protection; provide ventilation when dust may be generated.
HNOC	Chemical and toxicological properties may not be fully characterized.
Unknown acute toxicity	Not applicable - substance, not a mixture.

Section 3 - Composition / Information on Ingredients	
Substance / mixture	Substance
Chemical name	DOTA-tris(t-butyl ester); tri-tert-butyl protected DOTA with one free acetate carboxyl
CAS No.	137076-54-1
Molecular formula	C28H52N4O8
Molecular weight	572.73 g/mol
Purity / concentration	Product-specific; refer to Certificate of Analysis (COA).
Hazard-contributing impurities	No additional hazard-contributing impurities identified in the information reviewed for this document.

Section 4 - First-Aid Measures

Inhalation: Move to fresh air. Obtain medical attention if symptoms occur or persist. Skin contact: Remove contaminated clothing and wash thoroughly with soap and water. Eye contact: Rinse cautiously with water for several minutes; remove contact lenses if present and easy to do. Continue rinsing and obtain medical advice if irritation persists. Ingestion: Rinse mouth. Do not induce vomiting unless directed by medical personnel. Obtain medical advice if unwell. Treat symptomatically and supportively.

Section 5 - Fire-Fighting Measures

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide as appropriate for the surrounding fire. Specific hazards: Carbon oxides and nitrogen oxides may form during combustion; sulfur oxides may form for sulfur-containing compounds; fluorinated decomposition products may be relevant for TFA-containing material. Firefighter protection: Wear self-contained breathing apparatus and appropriate protective equipment when conditions warrant.

Section 6 - Accidental Release Measures

Avoid dust formation and inhalation. Provide ventilation and use appropriate personal protective equipment. Collect dry material carefully without generating dust and place in a suitable closed container for disposal. Prevent unnecessary release to drains or the environment.

Section 7 - Handling and Storage

Handle using good laboratory practice. Avoid inhalation of dust and unnecessary contact with skin and eyes. Keep container tightly closed and protect from contamination and moisture. Keep tightly closed, dry and cool. Follow lot-specific storage and handling information. Keep away from incompatible materials such as strong oxidizing agents unless supplier data indicate otherwise.

Section 8 - Exposure Controls / Personal Protection

Occupational exposure limits	No substance-specific OSHA PEL or ACGIH TLV identified in the information reviewed.
Engineering controls	Use general laboratory ventilation; local exhaust is appropriate where dust is generated.
Eye / face protection	Safety glasses or suitable chemical splash protection.
Skin / body protection	Suitable chemical-resistant gloves and laboratory clothing.
Respiratory protection	Normally not required under controlled handling; if dust is generated and ventilation is insufficient, use an appropriate NIOSH-approved particulate respirator.
Hygiene measures	Wash hands after handling. Do not eat, drink or smoke in chemical handling areas.

Section 9 - Physical and Chemical Properties

Physical state	Solid
Appearance	Solid/powder; lot appearance may vary
Odor	No data available
pH	No data available
Melting point	No validated Alan Scientific lot-specific value assigned in this document
Boiling point / range	No data available
Flammability	No data available
Flash point	No data available
Vapor pressure	No data available
Density / relative density	No validated lot-specific value assigned
Solubility	Product-specific; consult technical data/COA if available
Partition coefficient	No data available
Molecular weight	572.73 g/mol

Section 10 - Stability and Reactivity

Reactivity: No comprehensive reactivity data available. Chemical stability: Expected to be stable under recommended storage conditions. Hazardous reactions: No hazardous polymerization is known. Conditions to avoid: Excessive heat, moisture where relevant, and conditions inconsistent with recommended storage. Incompatible materials: Strong oxidizing agents unless product-specific data indicate otherwise. Hazardous decomposition products: Carbon oxides and nitrogen oxides may form during combustion; sulfur or fluorine-containing decomposition products may be possible where relevant to composition.

Section 11 - Toxicological Information

Likely exposure routes	Inhalation of dust, eye contact, skin contact and ingestion.
Acute toxicity	See Section 2. Numerical LD50/LC50 data are not assigned unless supported by reviewed source data.
Skin corrosion / irritation	See Section 2.
Eye damage / irritation	See Section 2.
Respiratory / skin sensitization	No data available.
Germ cell mutagenicity	No data available.
Carcinogenicity	Not identified here as a listed carcinogen by IARC, NTP or OSHA based on currently reviewed information.
Reproductive toxicity	No data available.
STOT - single exposure	See Section 2.
STOT - repeated exposure	No data available.
Aspiration hazard	Not applicable to the supplied solid based on available information.
Additional information	Chemical and toxicological properties may not be fully characterized. Handle using good laboratory safety practice.

Section 12 - Ecological Information

Ecotoxicity: No complete product-specific data available. Persistence / degradability: No data available. Bioaccumulation: No data available. Mobility in soil: No data available. Avoid unnecessary environmental release.

Section 13 - Disposal Considerations

Dispose of product, residues and contaminated packaging in accordance with applicable federal, state and local requirements. Do not mix with incompatible waste streams. Handle uncleaned containers as product residue.

Section 14 - Transport Information

Transport status	No dangerous-goods classification assigned in this document; verify shipment-specific carrier and jurisdictional requirements.
UN number	Not assigned in this document unless a regulated classification is confirmed.
Proper shipping name	Not assigned.
Hazard class	Not assigned.
Packing group	Not assigned.
Environmental hazards	No transport-specific environmental classification assigned in this document.
Special precautions	Use secure, closed packaging appropriate for laboratory chemicals and verify carrier requirements before shipment.

Section 15 - Regulatory Information

OSHA HCS	Prepared with consideration of the OSHA Hazard Communication Standard (29 CFR 1910.1200); hazard classification is stated in Section 2 based on currently reviewed source information.
Other regulatory considerations	Users and importers are responsible for confirming TSCA, state, local and jurisdiction-specific requirements for the specific transaction and use.

Section 16 - Other Information

Revision	1.0
Date of preparation / revision	2026-09-06
Revision summary	Initial Alan Scientific MSDS for DOTA-tris(tBu ester) (AS2119) using the current 16-section product-document format.
Data / assessment basis	Alan Scientific product information; currently available supplier safety documentation and public chemical records reviewed for identity and hazard context. Final release should remain aligned with the lot-specific upstream supplier MSDS and COA.

Safety information notice: Information is provided in good faith for safe handling of the supplied research material and is based on information reasonably available as of the revision date. It is not a product specification or warranty. Users are responsible for determining suitability, controls and regulatory obligations for their specific use.