Safety Data Sheet

tert-Butyl Acetate-d_{12}

Section 1. Chemical product and company identifications

Product code: D-5517
Chemical formula: $C_6D_{12}O_2$
CAS: 358731-05-2
CAS (unlabelled): 540-88-5
Synonyms: Acetic Acid *tert*-Butyl Ester

Supplier / Manufacturer:

C/D/N Isotopes Inc.
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Website: www.cdnisotopes.com

In case of emergency:

TOXYSCAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Liquid
Warning: Highly flammable liquid and vapour.
Routes of entry: Inhalation, ingestion, skin and eyes

GHS (Globally Harmonized System of Classification and Labelling of Chemicals):

GHS Classification: - Flammable liquids (Category 2)

GHS Label elements: - Pictograms:

- Signal word: Danger

Hazards statement: - H225 Highly flammable liquid and vapour.

Precautionary statement: - P210 Keep away from heat/ hot surfaces/ sparks/ open flames/ ignition sources. No smoking.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
tert-Butyl Acetate-d_{12}	358731-05-2	> 98

Section 4. First aid measures

Eye contact: Flush eyes with water as a precaution.
Skin contact: Wash off with soap and plenty of water. Consult a physician.
Inhalation: If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
Ingestion: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.
General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

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Section 5. Firefighting measures

Flammability of the product: Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.
Lower explosion limit: 1.7 Vol%
Upper explosion limit: 9.8 Vol%
Auto-ignition temperature: No data available.
Flash point: 4 °C (39 °F)
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.
Firefighting media and instructions: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
Special protective equipment for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

Section 6. Accidental release measures

Personal precautions: Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition.
Environmental precautions: Do not let product enter drains.
Methods for cleaning up: Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Provide appropriate exhaust ventilation. Keep away from sources of ignition - No smoking. Take measures to prevent the build-up of electrostatic charge.
Storage: Store at room temperature. Adequate ventilation. Protect from heat and ignition sources.

Section 8. Exposure Controls, Personal Protections

Engineering controls: Use mechanical exhaust or laboratory fumehood to avoid exposure.
Eyes: Safety glasses with side-shields conforming to NIOSH (US) or EN 166 (EU).
Respiratory: Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US).
Hands: Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.
Skin/body: Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Section 9. Physical and chemical properties (unlabelled)

Molecular weight: 116.16 g/mol
Physical status: Liquid
Color: Colorless
Odour: No data available
Density: 0.866 g/cm^3
Melting point: -62 °C (-80 °F)
Boiling point: 97 - 98 °C (207 - 208 °F)
Vapour pressure: 56 hPa (42 mmHg) at 20 °C (68 °F)
Vapour density: 4 (Air = 1)
Partition coefficient (octanol/water): log Pow: 1.76
Water solubility: 8.3 g/L

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.
Incompatibility: Strong oxidizing agents.
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.
Reactivity conditions: Heat, flames and sparks

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Section 11. Toxicological information (unlabelled)

Toxicological data: *tert*-Butyl Acetate

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
tert-Butyl Acetate	540-88-5	Oral - Rat - 4,100 mg/kg Dermal - Rabbit - > 2,000 mg/kg	Inhalation - Rat - 4 h - > 2,230 mg/m^3

Potential acute effects

- **Eyes:** May cause eye irritation.
- **Skin:** May be harmful if absorbed through skin. May cause skin irritation.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** May be harmful if swallowed.

Potential chronic effects

- **Carcinogenic effects:** IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- **Mutagenic effects:** No data available.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
tert-Butyl Acetate	240 mg/l LC50 350 mg/l EC50	Oncorhynchus mykiss Daphnia magna	96 h 48 h

Effects on environment: No data available.
Mobility: No data available.
Environmental precautions: No data available.
Persistence and degradability: Result: 50 % - Inherently biodegradable.
Bioaccumulative potential: No data available.

Section 13. Disposal considerations

Waste disposal: Contact a licensed professional waste disposal service to dispose of this material.

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: Butyl acetates
UN number: UN1123
Class: 3
Packaging group: II

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 0
Flammable: 3
Reactivity: 0
Special conditions: None

Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous

U.S. Federal regulations:

TSCA 8(b) inventory: *tert*-Butyl Acetate
SARA 302/304/311/312 extremely hazardous substances: Not Listed
SARA 302/304 emergency planning and notification: Not Listed
SARA 302/304/311/312 hazardous chemicals: Not Listed
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard: Not Listed
CWA (Clean Water Act) 307: Not Listed
CWA (Clean Water Act) 311: Not Listed
CAA (Clean Air Act) 112 accidental release prevention: Not Listed
CAA (Clean Air Act) 112 regulated flammable substances: Not Listed
CAA (Clean Air Act) 112 regulated toxic substances: Not Listed

State regulations:

DEA List I Chemicals (Precursor Chemicals): Not Listed
DEA List II Chemicals (Essential Chemicals): Not Listed
Substances in Massachusetts: Not Listed
Dangerous substances in New Jersey: Not Listed
New York – Dangerous substances with acute effects: Not Listed
Dangerous substances in Pennsylvania – right to know: Not Listed

WHMIS (Canada):

B2 - Flammable liquid

Section 16. Additional information

References:

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part1910.1200 OSHA MSDS Requirements.
- 49CFR Table List of Hazardous Materials, UN#, Proper Shipping Names, PG. -Canada
- Gazette Part II, Vol. 122, No. 2 Registration SOR/88-64 31 December, 1987 Hazardous Products Act "Ingredient Disclosure List".
- Federal act on the controlled products
- Canadian Transport of Dangerous Goods, Regulations and Schedules, Clear Language version 2002.
- Toxicological repertory, HSC.
- Material safety data sheet from the components.

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Elaborated by: **Toxyscan Inc., 1-866-780-0599**
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