

## SAFETY DATA SHEET

Version 6.10  
Revision Date 05/16/2025  
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## SECTION 1. IDENTIFICATION

## 1.1 Product identifiers

Product name :  $\alpha,\alpha$ -Dimethylphenethyl butyrate

Product Number : W239402

Brand : Aldrich

CAS-No. : 10094-34-5

## 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

## 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

## 1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

## SECTION 2. HAZARDS IDENTIFICATION

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

Skin irritation : Category 2

Short-term (acute) aquatic hazard : Category 3

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Long-term (chronic) aquatic hazard : Category 3

### Other hazards

None known.

### GHS label elements

Hazard pictograms :



Signal Word : Warning

Hazard Statements : H315 Causes skin irritation.  
H412 Harmful to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**  
P264 Wash skin thoroughly after handling.  
P273 Avoid release to the environment.  
P280 Wear protective gloves.  
**Response:**  
P302 + P352 IF ON SKIN: Wash with plenty of water.  
P332 + P313 If skin irritation occurs: Get medical advice/ attention.  
P362 + P364 Take off contaminated clothing and wash it before reuse.  
**Disposal:**  
P501 Dispose of contents/ container to an approved waste disposal plant.

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## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

### Components

| Chemical name                                   | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|-------------------------------------------------|-------------------|-----------------------|--------------|
| $\alpha$ , $\alpha$ -Dimethylphenethyl butyrate | 10094-34-5*       | $\geq 80 - \leq 100$  | TSC          |

\* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

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## SECTION 4. FIRST AID MEASURES

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE  
SIGMA**

|                                                             |                                                                                                                       |
|-------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------|
| General advice                                              | : Show this safety data sheet to the doctor in attendance.                                                            |
| If inhaled                                                  | : After inhalation: fresh air.                                                                                        |
| In case of skin contact                                     | : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.             |
| In case of eye contact                                      | : After eye contact: rinse out with plenty of water. Remove contact lenses.                                           |
| If swallowed                                                | : After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.                  |
| Most important symptoms and effects, both acute and delayed | : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11 |
| Protection of first-aiders                                  | : For personal protection see section 8.                                                                              |
| Notes to physician                                          | : No data available                                                                                                   |

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## SECTION 5. FIREFIGHTING MEASURES

|                                       |                                                                                |
|---------------------------------------|--------------------------------------------------------------------------------|
| Suitable extinguishing media          | : Foam<br>Carbon dioxide (CO <sub>2</sub> )<br>Dry powder                      |
| Unsuitable extinguishing media        | : For this substance/mixture no limitations of extinguishing agents are given. |
| Specific hazards during fire fighting | : Combustible.                                                                 |

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

|                               |                 |
|-------------------------------|-----------------|
| Hazardous combustion products | : Carbon oxides |
|-------------------------------|-----------------|

|                                                |                                                                                                                                                                 |
|------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Specific extinguishing methods                 | : No data available                                                                                                                                             |
| Further information                            | : Prevent fire extinguishing water from contaminating surface water or the ground water system.                                                                 |
| Special protective equipment for fire-fighters | : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing. |

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

|                                                                     |                                                                                                                                                                                                                                                                                                    |
|---------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Personal precautions, protective equipment and emergency procedures | : Advice for non-emergency personnel:<br>Do not breathe vapours, aerosols.<br>Avoid substance contact.<br>Ensure adequate ventilation.<br>Evacuate the danger area, observe emergency procedures, consult an expert.<br>Advice for emergency responders:<br>For personal protection see section 8. |
| Environmental precautions                                           | : Do not let product enter drains.                                                                                                                                                                                                                                                                 |
| Methods and materials for containment and cleaning up               | : Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10).<br>Take up with liquid-absorbent material (e.g. Chemizorb® ). Dispose of properly. Clean up affected area.                                                                     |

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

|                                           |                                                      |
|-------------------------------------------|------------------------------------------------------|
| Further information on storage conditions | : Tightly closed.                                    |
| Storage class                             | : 10, Combustible liquids                            |
| Recommended storage temperature           | : Recommended storage temperature see product label. |
| Packaging material                        | : Suitable material: Amber Glass Bottle/Jar          |

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

Color : No data available

Odor : No data available

|                                                     |                                                                                                |
|-----------------------------------------------------|------------------------------------------------------------------------------------------------|
| Odor Threshold                                      | : No data available                                                                            |
| pH                                                  | : No data available                                                                            |
| Freezing point                                      | : < -94 °F / < -70 °C<br>Method: Regulation (EC) No. 440/2008, Annex, A.1                      |
| Boiling point/boiling range                         | : 459 - 491 °F / 237 - 255 °C<br>Method: lit.                                                  |
| Flash point                                         | : 243 °F / 117 °C<br>(1,013 hPa)<br>Method: closed cup                                         |
| Evaporation rate                                    | : No data available                                                                            |
| Burning rate                                        | : No data available                                                                            |
| Upper explosion limit /<br>Upper flammability limit | : No data available                                                                            |
| Lower explosion limit /<br>Lower flammability limit | : No data available                                                                            |
| Vapor pressure                                      | : 85 hPa (77 °F / 25 °C)                                                                       |
| Relative vapour density                             | : No data available                                                                            |
| Relative density                                    | : No data available                                                                            |
| Density                                             | : 0.969 g/mL (77 °F / 25 °C)<br>Method: lit.                                                   |
| Solubility(ies)<br>Water solubility                 | : 0.01611 g/l (68 °F / 20 °C)<br>pH: 7<br>Method: OECD Test Guideline 105                      |
| Partition coefficient: n-<br>octanol/water          | : log Pow: 4.7 (77 °F / 25 °C)<br>Method: OECD Test Guideline 117<br>Potential bioaccumulation |
| Autoignition temperature                            | : 802 °F / 428 °C (1,013 hPa)<br>Method: Regulation (EC) No. 440/2008, Annex, A.15             |
| Decomposition<br>temperature                        | : No data available                                                                            |
| Viscosity, dynamic                                  | : No data available                                                                            |
| Viscosity, kinematic                                | : No data available                                                                            |
| Flow time                                           | : No data available                                                                            |

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|                          |                                |
|--------------------------|--------------------------------|
| Explosive properties     | : Not classified as explosive. |
| Oxidizing properties     | : none                         |
| Molecular weight         | : 220.31 g/mol                 |
| Particle characteristics |                                |
| Particle size            | : No data available            |

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## SECTION 10. STABILITY AND REACTIVITY

|                                    |                                                                                                                                                 |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| Reactivity                         | : Forms explosive mixtures with air on intense heating.<br><br>A range from approx. 15 Kelvin below the flash point is to be rated as critical. |
| Chemical stability                 | : The product is chemically stable under standard ambient conditions (room temperature) .                                                       |
| Possibility of hazardous reactions | : No data available                                                                                                                             |
| Conditions to avoid                | : Strong heating.                                                                                                                               |
| Incompatible materials             | : Strong oxidizing agents                                                                                                                       |
| Hazardous decomposition products   | : In the event of fire: see section 5                                                                                                           |

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - > 5,000 mg/kg

Inhalation: No data available

LD50 Dermal - Rabbit - > 5,000 mg/kg

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

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Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 476  
Result: negative  
Test Type: Ames test  
Test system: *S. typhimurium*  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 471  
Result: negative  
Test Type: in vitro assay  
Test system: human lymphoblastoid cells  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 487  
Result: negative

### **Carcinogenicity**

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.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **Reproductive toxicity**

No data available

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

Repeated dose toxicity - Rat - male and female - Oral - 28 d - No observed adverse effect level - 500 mg/kg  
Remarks: Subacute toxicity

RTECS: ET0130000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## **SECTION 12. ECOLOGICAL INFORMATION**

### **Ecotoxicity**

#### **Components:**

#### **$\alpha$ , $\alpha$ -Dimethylphenethyl butyrate:**

Toxicity to daphnia and : EC50 (*Daphnia magna* (Water flea)): 15.4 mg/l



other aquatic  
invertebrates

Exposure time: 48 h  
Test Type: static test  
Method: OECD Test Guideline 202  
GLP: yes

Toxicity to  
microorganisms

: EC50 (activated sludge): 637 mg/l  
Exposure time: 3 h  
Test Type: Respiration inhibition  
Method: OECD Test Guideline 209  
GLP: yes  
  
NOEC (activated sludge): 312.5 mg/l  
Exposure time: 3 h  
Test Type: Respiration inhibition  
Method: OECD Test Guideline 209  
GLP: yes

## **Persistence and degradability**

### **Components:**

#### **$\alpha$ , $\alpha$ -Dimethylphenethyl butyrate:**

Biodegradability : Inoculum: activated sludge  
Result: Readily biodegradable.  
Biodegradation: 79 %  
Exposure time: 28 d  
Method: OECD Test Guideline 301F  
GLP: yes

## **Bioaccumulative potential**

### **Components:**

#### **$\alpha$ , $\alpha$ -Dimethylphenethyl butyrate:**

Partition coefficient: n- : log Pow: 4.7 (77 °F / 25 °C)  
octanol/water Method: OECD Test Guideline 117  
Remarks: Potential bioaccumulation

## **Mobility in soil**

No data available

## **Other adverse effects**

### **Product:**

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part  
82 Protection of Stratospheric Ozone - CAA Section  
602 Class I Substances  
Remarks: This product neither contains, nor was  
manufactured with a Class I or Class II ODS as  
defined by the U.S. Clean Air Act Section 602 (40 CFR  
82, Subpt. A, App.A + B).

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14. TRANSPORT INFORMATION

### International Regulations

#### IATA-DGR

Not regulated as a dangerous good

#### IMDG-Code

Not regulated as a dangerous good

#### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

### National Regulations

#### 49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

### Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

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## SECTION 15. REGULATORY INFORMATION

### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard

**SARA 313**

: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

**Clean Water Act**

This product does not contain any Hazardous Substances listed under the U.S. Clean Water Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. Clean Water Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

**US State Regulations****Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The components of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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**SECTION 16. OTHER INFORMATION****Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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