SAFETY DATA SHEET

Version 5.5 Revision Date 12/22/2015 Print Date 11/18/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : α,α -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

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich

3050 Spruce Street SAINT LOUIS MO 63103

USA

Telephone : +1 800-325-5832 Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin irritation (Category 2), H315 Skin sensitisation (Category 1), H317 Acute aquatic toxicity (Category 2), H401 Chronic aquatic toxicity (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word Warning

Hazard statement(s)

H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.

P264 Wash skin thoroughly after handling.

P272 Contaminated work clothing should not be allowed out of the workplace.

P273 Avoid release to the environment.

P280 Wear protective gloves.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

Aldrich - W239402 Page 1 of 7

P321 Specific treatment (see supplemental first aid instructions on this label).

P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.

P362 Take off contaminated clothing and wash before reuse.

P391 Collect spillage.

P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula : C₁₄H₂₀O₂

Molecular weight : 220.31 g/mol

CAS-No. : 10094-34-5

EC-No. : 233-221-8

Hazardous components

Component	Classification	Concentration
α, α-Dimethylphenethyl butyrate		
	Skin Irrit. 2; Skin Sens. 1;	<= 100 %
	Aquatic Acute 2; Aquatic	
	Chronic 2; H315, H317, H411	

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

Aldrich - W239402 Page 2 of 7

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

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

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm Break through time: > 480 min

Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 36 min

Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

Aldrich - W239402 Page 3 of 7

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose 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) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Form: liquid a) Appearance b) Odour No data available Odour Threshold No data available No data available d) e) Melting point/freezing No data available point

Initial boiling point and

237 - 255 °C (459 - 491 °F) - lit.

boiling range

g) Flash point 110 °C (230 °F) - closed cup

h) Evaporation rate No data available i) Flammability (solid, gas) No data available Upper/lower No data available j)

flammability or explosive limits

k) Vapour pressure No data available Vapour density No data available

m) Relative density 0.969 g/mL at 25 °C (77 °F)

n) Water solubility No data available No data available Partition coefficient: noctanol/water

Auto-ignition temperature

No data available

Decomposition temperature

No data available

No data available Viscosity No data available s) Explosive properties No data available Oxidizing properties

9.2 Other safety information

No data available

Aldrich - W239402 Page 4 of 7

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - No data available

In the event of fire: see section 5

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 sensitisation

The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

Germ cell mutagenicity

No data available

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.

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.

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 identified as a

carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Aldrich - W239402 Page 5 of 7

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: ET0130000

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

UN number: 3082 Class: 9 Packing group: III EMS-No: F-A, S-F

Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (α , α -Dimethylphenethyl

butyrate)

Marine pollutant:yes

IATA

UN number: 3082 Class: 9 Packing group: III

Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (α, α-Dimethylphenethyl butyrate)

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

Aldrich - W239402 Page 6 of 7

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.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

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

Pennsylvania Right To Know Components

CAS-No. Revision Date

 α , α -Dimethylphenethyl butyrate 10094-34-5

New Jersey Right To Know Components

CAS-No. Revision Date

α, α-Dimethylphenethyl butyrate 10094-34-5

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute Acute aquatic toxicity
Aquatic Chronic Chronic aquatic toxicity
H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H401 Toxic to aquatic life.

H411 Toxic to aquatic life with long lasting effects.

Skin Irrit. Skin irritation

HMIS Rating

Health hazard: 3
Chronic Health Hazard:
Flammability: 1
Physical Hazard 0

NFPA Rating

Health hazard: 3
Fire Hazard: 1
Reactivity Hazard: 0

Further information

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Preparation Information

Sigma-Aldrich Corporation Product Safety – Americas Region 1-800-521-8956

Version: 5.5 Revision Date: 12/22/2015 Print Date: 11/18/2018

Aldrich - W239402 Page 7 of 7