

Safety Data Sheet

Section 1. Identification of the substance/mixture and of the company/undertaking

Product identifier:

Product name: Methyl 3-oxobutanoate

Reference number(SDS): 22095jis_J_E1-1

Product type:

Reagent

Recommended use of the chemical and restrictions on use

Recommended uses: Research and Development

Restrictions on uses: Do not use for other purposes.

Details of the supplier of the safety data sheet

Manufacturer/Supplier: JUNSEI CHEMICAL CO., LTD.

Address: 1-6, Ohmano-cho, Koshigaya-shi, Saitama 343-0844, Japan

Division: Quality Assurance Department

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Section 2. Hazards identification

Classification of the substance or mixture

PHYSICAL AND CHEMICAL HAZARDS

Flammable liquids: Category 4

HEALTH HAZARDS

Serious eye damage/eye irritation: Category 2

Specific target organ toxicity – single exposure: Category 3 (Narcotic effects)

(Note) GHS classification without description: Not classified/Classification not possible

Label elements

Hazard pictograms:



Signal word: Warning

Hazard statements

H227-Combustible liquid

H319-Causes serious eye irritation

H336-May cause drowsiness or dizziness

Precautionary statements

Prevention

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Avoid breathing dust/fume/gas/mist/vapors/spray.

Use only outdoors or in a well-ventilated area.

Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

Wash hands thoroughly after handling. Do not touch eyes.

Response

In case of fire: Use alcohol-resistant foam, dry powder, CO2 to extinguish.

Get medical help if you feel unwell.

IF INHALED: Remove person to fresh air and keep comfortable for breathing.

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if

Methyl 3-oxobutanoate, JUNSEI CHEMICAL CO., LTD., 22095jis_J_E1-1, 17/Jun/2026

present and easy to do. Continue rinsing.

If eye irritation persists: Get medical help.

Storage

Store in a well-ventilated place. Keep container tightly closed.

Store locked up.

Disposal

Dispose of contents/container in accordance with local/regional/national/international regulations.

Section 3. Composition/information on ingredients

Substance/mixture:

Substance

Common name, synonyms: Methyl acetoacetate

Ingredient name: Methyl 3-oxobutanoate

Content (%): 98.0 <

Chemical formula: C₅H₈O₃

ENCS: 2-1474; 2-1475

CAS No.: 105-45-3

MW: 116.12

EC No.: 203-299-8

Note : The figures shown above are not the specifications of the product.

Section 4. First aid measures

Descriptions of first aid measures

General measures

Get medical help if you feel unwell.

IF INHALED

IF INHALED: Remove person to fresh air and keep comfortable for breathing.

Get medical help if you feel unwell.

IF INHALED: Get medical help.

IF ON SKIN

IF ON SKIN: Take off immediately all contaminated clothing. Immediately rinse with water for several minutes.

If skin irritation or rash occurs: Get medical help.

IF IN EYES

IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

If eye irritation persists: Get medical help.

IF SWALLOWED

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

If victim is conscious, give 1 – 2 glasses of water.

IF SWALLOWED: Get medical help.

Most important symptoms and effects, both acute and delayed

(Symptoms when inhalation or ingestion)

Headache. Drowsiness. Cough. Dizziness. Sore throat.

(Symptoms when skin and/or eye contact)

Conjunctival redness of the eyes. Pain of the eyes

Indication of any immediate medical attention and special treatment needed

Information on indication of any immediate medical attention and special treatment needed is not available.

Section 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

In case of fire, use alcohol-resistant foam, dry powder, CO2 to extinguish.

Unsuitable extinguishing media

Unsuitable extinguishing media data is not available.

Specific hazards arising from the substance or mixture

Containers may explode when heated.

Fire may produce irritating, corrosive and/or toxic gases.

Runoff from fire control or dilution water may cause pollution.

Advice for firefighters

Special extinguishing method

Evacuate non-essential personnel to safe area.

Special protective equipment and precautions for fire-fighters

Wear fire resistant or flame retardant clothing.

Wear protective gloves/protective clothing/eye protection/face protection.

Firefighters should wear self-contained breathing apparatus with a full facepiece operated in the positive pressure mode.

Section 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Ventilate area until material pick up is complete.

Wear proper protective equipment.

Environmental precautions

Avoid release to headsprings, rivers, lakes, ocean and groundwater.

Methods and materials for containment and cleaning up

Absorb spill with inert material (dry sand, earth, etc.), then place in a chemical waste container.

Preventive measures for secondary accident

Collect spillage.

Reference to other sections

Refer to section 8

Refer to section 13

Section 7. Handling and storage

Engineering measures

(Measures to prevent operator exposure)

Avoid breathing dust/fume/gas/mist/vapors/spray.

(Measures to prevent fire and explosion)

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

(Local ventilation/general ventilation)

Exhaust/ventilator should be available.

(Precautions)

Avoid contact with skin.

Avoid contact with eyes.

Advice on safe handling

Use only outdoors or in a well-ventilated area.

Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

Use personal protective equipment as required.

When using do not eat, drink or smoke.

Avoidance of contact

See Section 10: Stability and Reactivity.

Advice on general occupational hygiene

- Do not get in eyes, on skin, or on clothing.
- Wash hands thoroughly after handling. Do not touch eyes.
- Do not eat, drink or smoke when using this product.

Conditions for safe storage

- Keep container tightly closed.
- Keep cool.
- Store in accordance with local/regional/national/international regulations regulation.
- Store locked up.
- Protect from sunlight. Store in a well-ventilated place.

Incompatible substances

- Refer to Section 10. Stability and reactivity.

Container and packaging materials for safe handling data is not available.

Specific end use(s)

- See information in Section 7.1 and 7.2 for handling and storage recommendations. See Section 8 for exposure controls and personal protection recommendations.

Section 8. Exposure controls/personal protection**Permissible concentration****Control value and Concentration standard value under ISHA**

- Not established

Occupational exposure limit values**JSOH**

- Not established

ACGIH

- Not established

Exposure controls**Appropriate engineering controls**

- Do not use in areas without adequate ventilation.
- Eye wash station should be available.
- Washing facilities should be available.

Individual protection measures, such as personal protective equipment**Respiratory protection**

- Select and wear respiratory protection in accordance with approved standards (e.g. JIS T8150).
- Recommended respiratory protection: Gas mask

Hand protection

- Wear protective gloves. Recommended material(s): butyl rubber
- Inspect before use and replace worn or damaged gloves.
- Contact the glove manufacturer for specific advice on glove selection and breakthrough times for your use conditions.
- Chemical-resistant, impervious gloves complying with an approved standard (e.g. JIS T8116) should be used.

Eye/face protection

- Wear chemical safety goggle.
- Wear eye/face protection in accordance with approved standards (e.g. JIS T8147).

Skin and body protection

- Wear impervious clothing and boots in case of repeated or prolonged treatment.
- Personal protective equipment for the body and skin should be selected based on the task being performed and the risks involved.

Section 9. Physical and Chemical Properties

Information on basic physical and chemical properties

Physical state: Liquid

Color: Colorless

Odor: Characteristic odor

Odor threshold data is not available.

Melting point/Freezing point: -27°C

Boiling point or initial boiling point and boiling range: 171.7°C

Flammability: Ignitable

Lower and upper explosion limit:

Lower explosion limit: 1.4 vol %

Upper explosion limit: 14.5 vol %

Flash point: 77°C (Closed cup)

Auto-ignition temperature: 280°C

Decomposition temperature data is not available.

pH data is not available.

Kinematic viscosity data is not available.

Solubility:

Solubility in water: 500g/liter

Solubility in solvent: Miscible with alcohol and ether.

Partition coefficient n-octanol/water (log value): -0.26

Vapor pressure: 0.17 kPa (20°C)

Density and/or relative density: $1.074 \sim 1.079 \text{ g/mL} (20^{\circ}\text{C})$

Relative vapor density (Air=1): 4.0

Relative density of the Vapor/air – mixture at 20°C (Air = 1): 1.01

Particle characteristics data is not available.

Section 10. Stability and Reactivity

Reactivity

Reactivity data is not available.

Chemical stability

Stable under normal storage/handling conditions.

Possibility of hazardous reactions

Decomposes on burning. This produces irritating fumes.

Reacts with oxidants.

Conditions to avoid

Avoid direct sunlight, fire, flame, high temperature.

Contact with incompatible materials.

Incompatible materials

Oxidizing agents

Hazardous decomposition products

Carbon oxides

Section 11. Toxicological Information

Information on toxicological effects

Acute toxicity

Acute toxicity (Oral)

[Product]

Based on available data, the classification criteria are not met.

[Data for components of the product]

[NITE-CHRIP]

rat : No mortality occurred in 2000 mg/kg groups. (OECD TG 401, GLP) (source: NITE)

Acute toxicity (Dermal)

[Product]

Based on available data, the classification criteria are not met.

[Data for components of the product]

[NITE-CHRIP]

rabbit LD50: > 5000 mg/kg (source: NITE)

Acute toxicity (Inhalation)

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

[NITE-CHRIP]

mist: rat LC50: > 6.6 mg/L (4-hour) (source: NITE)

Skin corrosion/irritation

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

No data available.

Serious eye damage/irritation

[Product]

Category 2, Causes serious eye irritation

[Data for components of the product]

[NITE-CHRIP]

Category 2 (source: NITE)

Respiratory or skin sensitization

Respiratory sensitization

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

No data available.

Skin sensitization

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

No data available.

Germ cell mutagenicity

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

No data available.

Carcinogenicity

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

No data available.

Reproductive toxicity

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

No data available.

Specific target organ toxicity – single exposure

[Product]

Category 3, May cause drowsiness or dizziness

[Data for components of the product]

[NITE-CHRIP]

Category 3 (Narcotic effects) (source: NITE)

Specific target organ toxicity – repeated exposure

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

No data available.

Aspiration hazard

[Product]

Classification not possible (Insufficient data available or no data available).

[Data for components of the product]

No data available.

Information on other hazards

[Data for components of the product]

No data available.

Section 12. Ecological Information

Ecotoxicity

Aquatic toxicity

[Product]

Based on available data, the classification criteria are not met.

[Data for components of the product]

Hazardous to the aquatic environment, short-term (acute)

[NITE-CHRIP]

Crustacea (*Daphnia magna*) 48-hour EC50: > 236.9 mg/L (source: NITE)Algae (*Pseudokirchneriella subcapitata*) 72-hour ErC50: > 978 mg/L (source: NITE)

Fish (Fathead minnow) 96-hour LC50: > 111.4 mg/L (source: NITE)

Water solubility

[Data for components of the product]

500 g/L (source: NITE)

Persistence and degradability

Persistence and degradability data is not available.

Bioaccumulative potential

[Data for components of the product]

log Pow: -0.26 (source: ICSC, 2003)

Mobility in soil

Mobility in soil data is not available.

Other adverse effects

Ozone depleting chemical data is not available.

Section 13. Disposal considerations

Waste treatment methods

Waste from residues

Disposal should be in accordance with local, national, and international laws and regulations.

Comply with relevant laws and regulations as well as local municipal standards.

Do not dump into sewers, on the ground or into any body of water.

Contaminated packing

Disposal should be in accordance with local, national, and international laws and regulations.

Comply with relevant laws and regulations as well as local municipal standards.

Dispose of container after using the contents completely.

Section 14. Transport Information

UNRTDG

UN number : Not regulated

UN Proper Shipping Name : Not regulated

Transport hazard class(es) : Not regulated

Packing group : Not regulated

IMDG Code (International Maritime Dangerous Goods Regulations)

UN number : Not regulated

UN Proper Shipping Name : Not regulated

Transport hazard class(es) : Not regulated

Packing group : Not regulated

IATA (Dangerous Goods Regulations)

UN number : Not regulated

UN Proper Shipping Name : Not regulated

Transport hazard class(es) : Not regulated

Packing group : Not regulated

Marine pollutants (yes/no) : no

Special precautions for user

No information available.

Maritime transport in bulk according to IMO instruments

MARPOL Annex II – Noxious Liquid Substances

Noxious Liquid Substances ; Cat. Z

Methyl 3-oxobutanoate

Section 15. Regulatory Information

Mutagenic Chemical Substances [MHLW_J Notice]

Methyl 3-oxobutanoate

U.S. Toxic Substances Control Act (TSCA) Inventory

Chemicals listed in TSCA Inventory

105-45-3

All components are listed or exempted.

Other regulatory information

We are not able to check up the regulatory information with regard to the substances in your country or region, therefore, we request this matter would be filled by your responsibility.

Regulatory information with regard to this substance in your country or in your region should be examined by your own responsibility.

Ensure this material in compliance with federal requirements and ensure conformity to local regulations.

Regulatory information in this section are limited to intentional ingredient(s), but does not contain information on non-intentional ingredients or impurities which are not informed by supplier(s).

Chemical safety assessment

Advice on safe handling for this product can be found in sections 7 and 8 of this SDS.

Section 16. Other information

GHS classification and labelling

H227-Flammable liquids, Category 4: H227 Combustible liquid

Methyl 3-oxobutanoate, JUNSEI CHEMICAL CO., LTD., 22095jis_J_E1-1, 17/Jun/2026

H319–Serious eye damage/eye irritation, Category 2: H319 Causes serious eye irritation

H336–Specific target organ toxicity – single exposure, Category 3, Narcotic effects: H336

May cause drowsiness or dizziness

References and sources for data

Globally Harmonized System of classification and labelling of chemicals, UN

Recommendations on the TRANSPORT OF DANGEROUS GOODS 23rd edit., 2023 UN

IMDG Code, 2024 Edition (Incorporating Amendment 42–24)

IATA Dangerous Goods Regulations (67th Edition) 2026

2024 EMERGENCY RESPONSE GUIDEBOOK (US DOT)

2026 TLVs and BEIs. (ACGIH)

JIS Z 7252 : 2025

JIS Z 7253 : 2025

Recommendation of occupational exposure limits (2024–2025) (JSOH)

Notification No. 0111–1 (January 11, 2022), Chemical Hazards Control Division, Industrial Safety and Health Department, Labour Standards Bureau, MHLW in Japan

Supplier's data/information

Chemicals safety data management system "GHS Assistant" Version 4.39 (<https://www.asahi-ghs.com/>)

NITE Chemical Risk Information Platform "NITE-CHRIIP"

(https://www.chem-info.nite.go.jp/en/chem/chrip/chrip_search/systemTop)

GHS Classification Guidance for Enterprises 2019 Revised Edition (Ver. 2.1) (May. 2024, METI)

Abbreviations and acronyms

ACGIH – American Conference of Governmental Industrial Hygienists;

anh – anhydride;

ATE – Acute Toxicity Estimate;

BCF – Bioconcentration Factor;

BOD – Biochemical Oxygen Demand;

Cat. – Category;

Ceiling-C – Ceiling value;

COD – Chemical Oxygen Demand;

CSCL – Chemical Substances Control Law in Japan;

DSEN – Dermal Sensitization;

EC No. – The European Community number;

EC50 – Effective Concentration 50;

ENCS – Existing and New Chemical Substances Inventory under CSCL

EPA – US Environmental Protection Agency;

EU – European Union;

GHS – Globally Harmonized System of Classification and Labelling of Chemicals;

IARC – International Agency for Research on Cancer;

IATA – International Air Transport Association;

IBC Code – International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk;

IMDG Code – International Maritime Dangerous Goods Code;

ISHA – Industrial Safety and Health Act in Japan;

JSOH – Japan Society for Occupational Health;

LC50 – Lethal Concentration 50;

LD50 – Lethal Dose 50;

logPow – n-Octanol/water Partition Coefficient;

MARPOL – International Convention for the Prevention of Pollution from Ships;

METI – Ministry of Economy, Trade and Industry in Japan;

MHLW – Ministry of Health, Labour and Welfare in Japan;

MOE – Ministry of the Environment in Japan

NOEC – No Observed Effect Concentration;

NTP – US National Toxicology Program;

REACH – Registration, Evaluation, Authorisation and Restriction of Chemicals Regulation

(EC) No.1907/2006;

RSEN – Respiratory Sensitization;

Skin – Danger of cutaneous absorption;

STEL – Short-term Exposure Limit;

STOT – Specific target organ toxicity;

SVHC – Substance of Very High Concern under REACH;

TWA – time-weighted average;

UN – United Nations;

UNRTDG – United Nations Recommendations on the Transport of Dangerous Goods;

General Disclaimer

The information relates to this specific material. It may not be valid for this material, if used in combination with any other materials or in any process. It is the user's responsibility to satisfy him-selves as to the suitability and completeness of this information for his own particular use.

This data sheet was created based on the information we currently have and may be revised according to new information. In addition, the precautions apply only to normal handling, and in the case of special handling, please make adequate countermeasure to maintain your safety.

The data given here is based on current knowledge and experience. The purpose of this Safety Data Sheet is to describe the products in terms of their safety requirements. The data does not signify any warranty with regard to the products' properties.

The GHS classification data given here is based on current Data published in Japan (National Institute of Technology and Evaluation (NITE) Chemical Risk Information Platform (NITE-CHRIP), up to FY2024).