

3,5,5-Trimethyl-2-cyclohexen-1-one
JUNSEI CHEMICAL CO., LTD., 15315jis_J_E1-2, 27/May/2025

Date of issue for the 1st edition : 17/Jun/2015

Date of revision : 27/May/2025

Safety Data Sheet

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

Product identifier:

Product name: 3,5,5-Trimethyl-2-cyclohexen-1-one

Reference number(SDS):15315jis_J_E1-2

Product type:

Reagent

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

Relevant identified uses of the product: Research and Development

Uses advised against: 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

Telephone number: +81-48-986-6161

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e-mail address: shiyaku-t@junsei.co.jp

Section 2. Hazards identification

GHS classification and label elements of the product

Classification of the substance or mixture

PHYSICAL AND CHEMICAL HAZARDS

Flammable liquids: Category 4

HEALTH HAZARDS

Acute toxicity (Oral): Category 4

Acute toxicity (Dermal): Category 4

Serious eye damage/eye irritation: Category 2B

Carcinogenicity: Category 2

Specific target organ toxicity – single exposure: Category 3 (Respiratory tract irritation)

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

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

Label elements



Signal word: Warning

HAZARD STATEMENT

H227-Combustible liquid

H302-Harmful if swallowed

H312-Harmful in contact with skin

H320-Causes eye irritation

H351-Suspected of causing cancer

H335-May cause respiratory irritation



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H336-May cause drowsiness or dizziness

PRECAUTIONARY STATEMENT

Prevention

- Obtain special instructions before use.
- Do not handle until all safety precautions have been read and understood.
- 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.
- Wash contaminated parts thoroughly after handling.
- Wear protective gloves/protective clothing/eye protection/face protection.
- Do not eat, drink or smoke when using this product.

Response

- In case of fire: Use water mist, foam, dry powder, CO2 to extinguish.
- Specific treatment is required.
- IF exposed or concerned: Get medical advice/attention.
- Call a POISON CENTER/doctor/physician if you feel unwell.
- IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- IF ON SKIN: Wash with plenty of soap and water.
- Take off contaminated clothing and wash it before reuse.
- IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- If eye irritation persists: Get medical advice/attention.
- Rinse mouth.
- IF SWALLOWED: Call a POISON CENTER/doctor/physician if you feel unwell.

Storage

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

Disposal

- Dispose of contents/container in accordance with local/national regulation.

Specific Physical and Chemical hazards

- Heating may cause fire.

Section 3. Composition/information on ingredients

Mixture/Substance selection:

Substance

Common name, synonyms: Isophorone

Ingredient name:3,5,5-Trimethyl-2-cyclohexen-1-one

Content (%):(isomer mixtures) 98.0 <

Chemical formula:C9H14O

ENCS:3-2381;3-2389

CAS No.:78-59-1

MW:138.21

EC No.:201-126-0

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

Section 4. First-aid measures

Descriptions of first-aid measures

General measures

IF exposed or concerned: Get medical advice/attention.

Call a POISON CENTER/doctor/physician if you feel unwell.

IF INHALED

Remove person to fresh air and keep comfortable for breathing.

Call a POISON CENTER/doctor/physician if you feel unwell.

IF ON SKIN (or hair)

Take off immediately all contaminated clothing. Rinse skin with water or shower.

Wash with plenty of soap and water.

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

Call a POISON CENTER/doctor/physician if you feel unwell.

IF IN EYES

Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

If eye irritation persists: Get medical advice/attention.

IF SWALLOWED

Rinse mouth.

IF SWALLOWED: Call a POISON CENTER/doctor/physician if you feel unwell.

Give a slurry of activated charcoal in water to drink.

Most important symptoms and effects, both acute and delayed

(Symptoms when inhalation or ingestion)

Burning sensation. Sore throat. Cough. Dizziness. Headache. Nausea. Shortness of breath. Abdominal pain.

(Symptoms when skin and/or eye contact)

Redness of the eyes. Pain of the eyes. Blurred vision.

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

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Suitable extinguishing media

In case of fire, use water mist, 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

Specific fire-fighting measures

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

Personnel 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, et al), then place in a chemical waste container.

Collect leaking and spilled liquid in sealable containers as far as possible.

Preventive measures for secondary accident

Collect spillage.

Section 7. Handling and storage

Precautions for safe handling

Preventive measures

(Exposure Control for handling personnel)

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

(Protective measures against fire and explosion)

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

(Exhaust/ventilator)

Exhaust/ventilator should be available.

(Safety treatments)

Avoid contact with skin.

Avoid contact with eyes.

Safety Measures

Obtain special instructions before use.

Do not handle until all safety precautions have been read and understood.

Use only outdoors or in a well-ventilated area.

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

Use personal protective equipment as required.

When using do not eat, drink or smoke.

Any incompatibilities

Strong bases, Strong oxidizing agents, Amines should not be mixed with the chemicals.

Advice on general occupational hygiene

Wash contaminated parts thoroughly after handling.

Do not eat, drink or smoke when using this product.

Take off contaminated clothing and wash it before reuse.

Storage

Conditions for safe storage

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

Keep cool. Protect from sunlight.

Store in accordance with local/national regulation.

Store locked up.

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

Control parameters

Control value and Concentration standard value under ISHA

STEL: 5ppm

Occupational Exposure Limit

JSOH

Not established

ACGIH

Ceiling: 5ppm (Eye & URT irr; CNS impair; malaise; fatigue)

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

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

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T8116) should be used.

Eye protection

Wear safety glasses with side-shields.

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 ~ Light yellow

Odor: Characteristic odor

Odor threshold data is not available.

Melting point/Freezing point: -8°C

Boiling point or initial boiling point: 215°C

Boiling range data is not available.

Flammability (gases, liquids and solids) data is not available.

Lower and upper explosion limit/flammability limit:

Lower explosion limit: 0.8 vol %

Upper explosion limit: 3.8 vol %

Flash point: 84°C (C.C.)

Auto-ignition temperature: 460°C

Decomposition temperature data is not available.

Self-Accelerating Decomposition Temperature/SADT data is not available.

pH data is not available.

Dynamic viscosity: $2.62\text{mPa}\cdot\text{s}$ (20°C)

Kinematic viscosity data is not available.

Solubility:

Solubility in water: 1.2 g/100 mL (25°C)

Solubility in solvent data is not available.

n-Octanol/water partition coefficient: $\log P_{ow}1.67$

Vapor pressure: 40 Pa (20°C)

Vapor density data is not available.

Density and/or relative density: $0.920\sim 0.924\text{ g/mL}$ (20°C)

Relative vapor density (Air=1): 4.8

Relative density of the Vapor/air - mixture at 20°C (Air = 1) data is not available.

Particle characteristics data is not available.

Other information

Critical temperature data is not available.

Evaporation rate data is not available.

VOC data is not available.

Section 10. Stability and Reactivity

Reactivity

Reactivity data is not available.

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Chemical stability

Stable under normal storage/handling conditions.

Possibility of hazardous reactions

Reacts with strong oxidants, strong bases and amines.

Conditions to avoid

Contact with incompatible materials.

Open flames. Heating. Air.

Incompatible materials

Strong bases. Strong oxidizing agents. Amines.

Hazardous decomposition products

Carbon oxides.

Section 11. Toxicological Information

Information on toxicological effects

Acute toxicity

Acute toxicity (Oral)

[Product]

Category 4, Harmful if swallowed

[Data for components of the product]

[NITE-CHRIP]

rat LD50: 1500 mg/kg (source: NITE)

Acute toxicity (Dermal)

[Product]

Category 4, Harmful in contact with skin

[Data for components of the product]

[NITE-CHRIP]

rabbit LD50: 1200 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: 7000 mg/m³ (4-hour) (source: NITE)

Irritant properties

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 2B, Causes eye irritation

[Data for components of the product]

[NITE-CHRIP]

Category 2B (source: NITE)

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]

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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]

Category 2, Suspected of causing cancer

[Data for components of the product]

[NITE-CHRIP]

Category 2 (source: NITE)

[IARC]

2B: Possibly carcinogenic to humans

[ACGIH]

A3: Confirmed Animal Carcinogen with Unknown Relevance to Humans

[JSOH]

Group 2B: The agents which are probably or possibly carcinogenic to humans

[EU]

Category 2; Substances suspected human carcinogens

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 (STOT)

STOT-single exposure

[Product]

Category 3, May cause respiratory irritation

Category 3, May cause drowsiness or dizziness

[Data for components of the product]

[NITE-CHRIP]

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Category 3 (Respiratory tract irritation), Category 3 (Narcotic effects) (source: NITE)

STOT-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.

Section 12. Ecological Information

Ecotoxicity

Aquatic toxicity

[Product]

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

[Data for components of the product]

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

[NITE-CHRIP]

Fish (*Oryzias latipes*) 96-hour LC50: > 100 mg/L (OECD TG 203, GLP) (source: NITE)Crustacea (*Daphnia magna*) 48-hour EC50: 220 mg/L (source: NITE)Algae (*Raphidocelis subcapitata*) 72-hour ErC50: 230 mg/L (OECD TG 201, GLP) (source: NITE)

Hazardous to the aquatic environment, long-term (chronic)

[NITE-CHRIP]

Fish (*Pimephales promelas*) 32-day NOEC: 9.88 mg/L (source: NITE)Crustacea (*Daphnia magna*) 21-day NOEC: > 100 mg/L (OECD TG 202, GLP) (source: NITE)Algae (*Raphidocelis subcapitata*) 72-hour NOErC: 43 mg/L (OECD TG 201, GLP) (source: NITE)

Water solubility

[Data for components of the product]

1.2 g/100 mL (25°C) (source: ICSC, 2000)

Persistence and degradability

[Data for components of the product]

Rapidly degradable (Degradation rate: 95% (by DOC); passing the 10-day window

(EU Method C.4-A, GLP)) (source: NITE)

Bioaccumulative potential

[Data for components of the product]

log Pow: 1.67 (source: ICSC, 2000)

Mobility in soil

Mobility in soil data is not available.

Other adverse effects

Ozone depleting chemical data is not available.

Section 13. Disposal considerations

Description of waste residues and information on their safe handling and methods of disposal, including the disposal of any contaminated packaging

Waste treatment methods

Dispose of contents/container in accordance with local/national regulation.

Section 14. Transport Information

UN No., UN CLASS

UN Number or ID Number : Not regulated

UN Proper Shipping Name : Not regulated

Class or division (Transport hazard class) : Not regulated

Packing group : Not regulated

IMDG Code (International Maritime Dangerous Goods Regulations)

UN Number or ID Number : Not regulated

UN Proper Shipping Name : Not regulated

Class or division (Transport hazard class) : Not regulated

Packing group : Not regulated

IATA (Dangerous Goods Regulations)

UN Number or ID Number : Not regulated

UN Proper Shipping Name : Not regulated

Class or division (Transport hazard class) : Not regulated

Packing group : Not regulated

Environmental hazards

Marine pollutants (yes/no) : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Noxious Liquid Substances ; Cat. Y

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Section 15. Regulatory Information

Safety, health and environmental regulations/legislation specific for the substance or mixture

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

Chemicals listed in TSCA Inventory

78-59-1

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

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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

H302-Acute toxicity, Category 4: H302 Harmful if swallowed

H312-Acute toxicity, Category 4: H312 Harmful in contact with skin

H320-Serious eye damage/eye irritation, Category 2B: H320 Causes eye irritation

H351-Carcinogenicity, Category 2: H351 Suspected of causing cancer

H335-STOT – single exposure, Category 3, Respiratory tract irritation: H335 May cause respiratory irritation.

H336-STOT – 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 (66th Edition) 2025

2024 EMERGENCY RESPONSE GUIDEBOOK (US DOT)

2025 TLVs and BEIs. (ACGIH)

JIS Z 7252 : 2019

JIS Z 7253 : 2019

2024 Recommendation on TLVs (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 4.33

(<https://www.asahi-ghs.com/>)

NITE Chemical Risk Information Platform "NITE-CHRIP"

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

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

Abbreviations and acronyms

SDS (Safety Data Sheet)

LD50 (Lethal Dose, 50%)

LC50 (Lethal Concentration, 50%)

IARC (International Agency for Research on Cancer)

ACGIH (American Conference of Governmental Industrial Hygienists)

EPA (US Environmental Protection Agency)

NTP (US National Toxicology Program)

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)

JSOH (Japan Society for Occupational Health)

ISHA (Industrial Safety and Health Act in Japan)

CSCL (Chemical Substances Control Law in Japan)

EU (European Union)

EC50 (Effective Concentration, 50%)

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NOEC (No Observed Effect Concentration)

BOD (Biochemical Oxygen Demand)

COD (Chemical Oxygen Demand)

BCF (Bioconcentration Factor)

anh (anhydride)

General Disclaimer

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 FY2023).