

## Chemical Safety Data Sheet MSDS / SDS

**2,2,5-TRIMETHYLHEXANE**Revision Date:2023-06-10 Revision Number:1

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 2,2,5-TRIMETHYLHEXANE  
CBnumber : CB5735123  
CAS : 3522-94-9  
EINECS Number : 222-537-1  
Synonyms : 2,2,5-trimethylhexane,isononane

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

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**SECTION 2: Hazards identification****Classification of the substance or mixture**

Flammable liquids, Category 2

**Label elements****Pictogram(s)**

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Signal word : Danger

**Hazard statement(s)**

H225 Highly flammable liquid and vapour

**Precautionary statement(s)****Prevention**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

#### **Response**

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

#### **Storage**

P403+P235 Store in a well-ventilated place. Keep cool.

#### **Disposal**

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

#### **Other hazards**

no data available

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: 2,2,5-TRIMETHYLHEXANE
Synonyms	: 2,2,5-trimethylhexane,isononane
CAS	: 3522-94-9
EC number	: 222-537-1
MF	: C9H20
MW	: 128.26

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **If inhaled**

Fresh air, rest. Refer for medical attention.

#### **Following skin contact**

Rinse and then wash skin with water and soap. Refer for medical attention if skin irritation occurs.

#### **Following eye contact**

Rinse with plenty of water (remove contact lenses if easily possible).

#### **Following ingestion**

Rinse mouth. Do NOT induce vomiting. Refer for medical attention .

### **Most important symptoms and effects, both acute and delayed**

no data available

### **Indication of any immediate medical attention and special treatment needed**

no data available

## SECTION 5: Firefighting measures

### Extinguishing media

Use foam, powder, carbon dioxide.

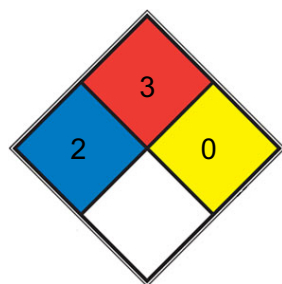
### Specific Hazards Arising from the Chemical

no data available

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 3 Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

SPEC.

HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Absorb remaining liquid in dry sand or inert absorbent. Then store and dispose of according to local regulations.

### Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws

and regulations.

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## SECTION 7: Handling and storage

### Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

### Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong oxidants. Store in an area without drain or sewer access.

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## SECTION 8: Exposure controls/personal protection

### Control parameters

#### Occupational Exposure limit values

no data available

#### Biological limit values

no data available

### Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### Individual protection measures

#### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

#### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

#### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Physical state	COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR.
Colour	no data available
Odour	no data available
Melting point/freezing point	320°C(dec.)(lit.)

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Boiling point or initial boiling point and boiling range	122°C
Flammability	Flammable.
Lower and upper explosion limit/flammability limit	no data available
Flash point	13°C(lit.)
Auto-ignition temperature	205°C
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	<7 mm <sup>2</sup> /s at 40°C
Solubility	In methanol, g/L: 162 at 5 °C, 179 at 10 °C, 200 at 15 °C, 221 at 20 °C, 247 at 25 °C, 280 at 30 °C, 316 at 35 °C, 360 at 40 °C (Kiser et al., 1961); miscible with hexane and pentane.
Partition coefficient n-octanol/water	5.65
Vapour pressure	3.647 at 0.000 °C, 5.072 at 5.000 °C, 6.958 at 10.000 °C, 9.418 at 15.000 °C, 12.583 at 20.000 °C, 16.625 at 25.000 °C, 21.719 at 30.000 °C (inclined-piston, Osborn and Douslin, 1974)
Density and/or relative density	0.71 g/cm <sup>3</sup>
Relative vapour density	(air = 1): 4.4
Particle characteristics	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Reacts with strong oxidants. This generates fire and explosion hazard.

### Chemical stability

no data available

### Possibility of hazardous reactions

As a result of flow, agitation, etc., electrostatic charges can be generated.

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

## SECTION 11: Toxicological information

### Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

**Skin corrosion/irritation**

no data available

**Serious eye damage/irritation**

no data available

**Respiratory or skin sensitization**

no data available

**Germ cell mutagenicity**

no data available

**Carcinogenicity**

no data available

**Reproductive toxicity**

no data available

**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

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## SECTION 12: Ecological information

**Toxicity**

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

**Persistence and degradability**

no data available

**Bioaccumulative potential**

no data available

### **Mobility in soil**

no data available

### **Other adverse effects**

no data available

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## **SECTION 13: Disposal considerations**

### **Disposal methods**

#### **Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### **Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## **SECTION 14: Transport information**

### **UN Number**

ADR/RID: UN3295 (For reference only, please check.)

IMDG: UN3295 (For reference only, please check.)

IATA: UN3295 (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

IMDG: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

IATA: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

### **Transport hazard class(es)**

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

### **Environmental hazards**

ADR/RID: No

IMDG: No

IATA: No

### **Special precautions for user**

no data available

### **Transport in bulk according to IMO instruments**

no data available

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## SECTION 15: Regulatory information

### **Safety, health and environmental regulations specific for the product in question**

#### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

#### **EC Inventory**

Listed.

#### **United States Toxic Substances Control Act (TSCA) Inventory**

Not Listed.

#### **China Catalog of Hazardous chemicals 2015**

Listed.

#### **New Zealand Inventory of Chemicals (NZIoC)**

Not Listed.

#### **PICCS**

Not Listed.

#### **Vietnam National Chemical Inventory**

Not Listed.

#### **IECSC**

Not Listed.

#### **Korea Existing Chemicals List (KECL)**

Listed.

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## SECTION 16: Other information

### **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%



EC50: Effective Concentration 50%

## References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pagenID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pagenID=0&request_locale=en)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

### Disclaimer:

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