Chemical Safety Data Sheet MSDS / SDS

2,4,4-trimethylpent-1-ene SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: 2,4,4-trimethylpent-1-ene

CAS: 107-39-1

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.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

Telephone: +91 9550333722

SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 2
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H411 Toxic to aquatic life with long lasting effects

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/...
P273 Avoid release to the environment.

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.
P391 Collect spillage.

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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	2,4,4-trimethylpent-1-ene
Common names and synonyms:	2,4,4-trimethylpent-1-ene
CAS number:	107-39-1
EC number:	203-486-4
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Give a slurry of activated charcoal in water to drink. Do NOT induce vomiting. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Low general toxicity; may act as simple asphyxiant in high vapor concentrations. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Foam, carbon dioxide, dry chemical ...

Specific hazards arising from the chemical

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. Substance may be transported hot. For hybrid vehicles, ERG Guide 147 (lithium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. If molten aluminum is involved, refer to ERG Guide 169. (ERG, 2016)

Special protective actions for fire-fighters

Use powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water. Combat fire from a sheltered position.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Personal protection: self-contained breathing apparatus. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Evacuate danger area! Personal protection: self-contained breathing apparatus. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in 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.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. Prevent build-up of electrostatic charges (e.g., by grounding). Do NOT use compressed air for filling, discharging, or 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. Cool. Keep in a well-ventilated room.STORAGE TEMPERATURE: AMBIENT; VENTING: OPEN (FLAME ARRESTER) OR PRESSURE-VACUUM.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering 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, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles or eye protection in combination with breathing protection.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Diisobutylene, isomeric compounds is a clear colorless liquid with a petroleum-like odor. Flash point 10°F. Less dense than water and insoluble in water. Vapors heavier than air. Used in the manufacture of other chemicals.
Colour:	Colorless liquid
Odour:	GASOLINE-LIKE ODOR
Melting point/freezing point:	-93°C(lit.)
Boiling point or initial boiling point and boiling range:	100°C
Flammability:	Highly flammable. Heating will cause rise in pressure with risk of bursting.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 0.8% by volume; Upper flammable limit: 4.8% by volume
Flash point:	-7°C(lit.)
Auto-ignition temperature:	788° F (USCG, 1999)
Decomposition temperature:	no data available
pH:	no data available

Kinematic viscosity:	no data available
Solubility:	Insoluble in water. Soluble in ethyl ether, benzene, carbon tetrachloride
Partition coefficient n-octanol/water:	log Kow= 4.55
Vapour pressure:	25.7mmHg at 25°C
Density and/or relative density:	0.719g/cm3
Relative vapour density:	3.8 (AIR= 1)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts violently with oxidants.
Reacts with oxidants.

Chemical stability

no data available

Possibility of hazardous reactions

FIRE HAZARD: DANGEROUS, WHEN EXPOSED TO HEAT OR FLAME; CAN REACT VIGOROUSLY WITH OXIDIZING MATERIALS.The vapour is heavier than air and may travel along the ground; distant ignition possible. As a result of flow, agitation, etc., electrostatic charges can be generated.,The vapour is heavier than air and may travel along the ground; distant ignition possible.DIISOBUTYLENE may react vigorously with strong oxidizing agents. May react exothermically with reducing agents to release hydrogen gas.

Conditions to avoid

no data available

Incompatible materials

Mixing diisobutylene /with chlorosulfonic acid, oleum, or 96% sulfuric acid/ ... in a closed container caused temperature & pressure to increase.

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

The substance is irritating to the eyes, skin and respiratory tract. Exposure to high concentrations could cause unconsciousness.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air can be reached very quickly on evaporation of this substance at 20°C.

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

2,2,4-Trimethyl-1-pentene is expected to biodegrade slowly in soil and water based upon no biodegradation in the Japanese MITI test(1).

Bioaccumulative potential

An estimated log BCF of 2.80 was calculated for 2,4,4-trimethyl-1-pentene(SRC), using an estimated log Kow of 4.55(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high.

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc for 2,4,4-trimethyl-1-pentene can be estimated to be about 275(SRC). According to a classification scheme(2), this estimated Koc value suggests that 2,4,4-trimethyl-1-

pentene is expected to have moderate mobility in soil.

Other adverse effects

no data available

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.

SECTION 14: Transport information

UN Number

ADR/RID: UN2050 (For reference only, please check.)
IMDG: UN2050 (For reference only, please check.)
IATA: UN2050 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: DIISOBUTYLENE, ISOMERIC COMPOUNDS (For reference only, please check.)
IMDG: DIISOBUTYLENE, ISOMERIC COMPOUNDS (For reference only, please check.)
IATA: DIISOBUTYLENE, ISOMERIC COMPOUNDS (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: II (For reference only, please check.)
IMDG: II (For reference only, please check.)
IATA: II (For reference only, please check.)

Environmental hazards

ADR/RID: Yes
IMDG: Yes
IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

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

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

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?pageID=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/

Other Information

Health effects of exposure to the substance have not been investigated.