

Chemical Safety Data Sheet MSDS / SDS

TRANS-1,3-PENTADIENERevision Date:2024-12-21 Revision Number:1

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

Product name : TRANS-1,3-PENTADIENE
CBnumber : CB6421102
CAS : 504-60-9
EINECS Number : 207-995-2
Synonyms : Piperylene,1,3-pentadiene

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

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

Flammable liquids, Category 2

Label elements**Pictogram(s)**

□

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

SECTION 3: Composition/information on ingredients

Substance

Product name	: TRANS-1,3-PENTADIENE
Synonyms	: Piperylene,1,3-pentadiene
CAS	: 504-60-9
EC number	: 207-995-2
MF	: C ₅ H ₈
MW	: 68.12

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. Seek medical attention if you feel unwell.

Following skin contact

Remove contaminated clothes. 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. Seek medical attention if you feel unwell.

Most important symptoms and effects, both acute and delayed

Vapors may cause dizziness or suffocation; contact may irritate skin and eyes. (USCG, 1999)

Indication of any immediate medical attention and special treatment needed

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock and treat if necessary . Anticipate seizures and

treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Aliphatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Extinguishing media

Water may be effective.

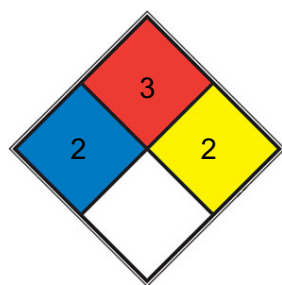
Specific Hazards Arising from the Chemical

Special Hazards of Combustion Products: Fire produces irritating and poisonous gases. Behavior in Fire: Will burn and produce irritating and poisonous gases. Container may explode in heat of fire. Vapor explosion hazard indoors, outdoors, or in sewers. Runoff to sewer may create fire or explosion hazard. (USCG, 1999)

Advice for firefighters

Use water spray, foam, powder, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

NFPA 704



<input checked="" type="checkbox"/> HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. diethyl ether , ammonium phosphate, iodine)
<input checked="" type="checkbox"/> 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)
<input checked="" type="checkbox"/> REACT	2	Undergoes violent chemical change at elevated temperatures and pressures, reacts violently with water, or may form explosive mixtures with water (e.g. white phosphorus, potassium , sodium)
<input type="checkbox"/> SPEC.		
<input type="checkbox"/> HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Remove all ignition sources. Evacuate danger area! Consult an expert! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Collect leaking liquid in covered containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

Environmental precautions

Remove all ignition sources. Evacuate danger area! Consult an expert! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Collect leaking liquid in covered containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

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. Do NOT use compressed air for filling, discharging, or handling. Use non-sparking handtools. 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

Separated from strong oxidants. Fireproof. Store in an area without drain or sewer access. Ventilation along the floor.

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 safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	1,3-pentadiene is a clear colorless liquid with an acrid odor. Flash point of -20°F. Boiling point 5°F. A dangerous fire risk. Vapors are irritating to the eyes and respiratory system. Subject to polymerization if heated or contaminated. If the polymerization takes place inside a container, the container may violently rupture. Insoluble in water. Used to make intermediates and polymers.
Colour	Colorless liquid
Odour	no data available
Melting point/freezing point	-87°C(lit.)
Boiling point or initial boiling point and boiling range	42°C(lit.)
Flammability	Highly flammable.
Lower and upper explosion limit/flammability limit	no data available
Flash point	<-30 °F
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	MISCIBLE WITH ALCOHOL, ETHER, ACETONE, BENZENE
Partition coefficient n-octanol/water	log Kow= 2.44
Vapour pressure	6.56 psi (20 °C)
Density and/or relative density	0.683 g/mL at 25°C(lit.)
Relative vapour density	2.4 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts violently with strong oxidants. Can form peroxides which may initiate a polymerisation reaction.

Chemical stability

no data available

Possibility of hazardous reactions

HIGHLY FLAMMABLE, DANGEROUS FIRE RISK. The vapour is heavier than air and may travel along the ground; distant ignition possible. 1,3-PENTADIENE may react vigorously with strong oxidizing agents. May react exothermically with reducing agents to release hydrogen gas. In the presence of various catalysts (such as acids) or initiators, may undergo exothermic addition polymerization reactions. May undergo autoxidation upon exposure to the air to form explosive peroxides. Violent explosions at low temperatures in ammonia synthesis units have been traced to the addition products of dienes and nitrogen dioxide [Bretherick, 5th Ed., 1995].

Conditions to avoid

no data available

Incompatible materials

Can react vigorously with oxidizing materials.

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

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 vapour is irritating to the eyes and skin. If swallowed the substance may cause vomiting and could result in aspiration pneumonitis. The effects may be delayed.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached 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

No biodegradation data regarding 1,3-pentadiene were located(SRC), however data on a similar compound, 1,3-butadiene are available(1-4). Laboratory studies employing pure bacterial cultures isolated from lake and soil samples were shown to degrade 1,3-butadiene to 1,2-epoxybutene, however it is not clear what the rate of degradation will be under environmental conditions(1-3). The biodegradation half-life of 1,3-butadiene in aerobic waters has been reported as 7 days and the half-life in anaerobic waters was reported as 28 days(4). These data suggest that 1,3-pentadiene will also undergo biodegradation under similar conditions(SRC).

Bioaccumulative potential

An estimated BCF of 15 was calculated for 1,3-pentadiene(SRC), using a log Kow of 2.44(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of 1,3-pentadiene is estimated as 500(SRC), using a log Kow of 2.44(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 1,3-pentadiene is expected to have low mobility in soil(SRC).

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: 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

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)

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

The commercial mixture of 1,3-pentadiene consists of 80% of the trans-isomer (CAS 2004-70-8) and 20% of the cis-isomer (CAS 1574-41-0).

CAS 504-60-9 is for unspecified or mixed isomer. Do NOT take working clothes home.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.