

1 Identification

Product identifier

Product name: 1,3,5-Trimethyl-1,4-cyclohexadiene

Stock number: H25921

CAS Number:

4074-23-1

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

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar

Thermo Fisher Scientific Chemicals, Inc.

30 Bond Street

Ward Hill, MA 01835-8099

Tel: 800-343-0660

Fax: 800-322-4757

Email: tech@alfa.com

www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS02 Flame

Flam. Liq. 3 H226 Flammable liquid and vapor.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS02

Signal word

Warning

Hazard statements

H226 Flammable liquid and vapor.

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P280 Wear protective gloves / eye protection / face protection.

P240 Ground/bond container and receiving equipment.

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

P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

B2 - Flammable liquid



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 1 Health (acute effects) = 1

FIRE 2 Flammability = 2

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

4074-23-1 1,3,5-Trimethyl-1,4-cyclohexadiene

Concentration: ≤100%

4 First-aid measures

Description of first aid measures

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm.

Seek immediate medical advice.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing Seek medical treatment.

Information for doctor

Most important symptoms and effects, both acute and delayed No further relevant information available.

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USA

Product name: 1,3,5-Trimethyl-1,4-cyclohexadiene

Indication of any immediate medical attention and special treatment needed No further relevant information available.

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5 Fire-fighting measures

Extinguishing media

Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Advice for firefighters

Protective equipment:

Wear self-contained respirator.

Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Keep away from ignition sources

Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.

Methods and material for containment and cleaning up:

Keep away from ignition sources.

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Prevention of secondary hazards: Keep away from ignition sources.

Reference to other sections

See Section 7 for information on safe handling

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

Protective Action Criteria for Chemicals

PAC-1: Substance is not listed.

PAC-2: Substance is not listed.

PAC-3: Substance is not listed.

7 Handling and storage

Handling

Precautions for safe handling

Keep container tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation at the workplace.

Information about protection against explosions and fires:

Protect against electrostatic charges.

Fumes can combine with air to form an explosive mixture.

Keep ignition sources away.

Conditions for safe storage, including any incompatibilities

Storage

Requirements to be met by storerooms and receptacles: No special requirements.

Information about storage in one common storage facility: Store away from oxidizing agents.

Further information about storage conditions:

Keep container tightly sealed.

Store in cool, dry conditions in well sealed containers.

Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace:

The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.

Additional information: No data

Exposure controls

Personal protective equipment

General protective and hygienic measures

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Maintain an ergonomically appropriate working environment.

Breathing equipment: Use suitable respirator when high concentrations are present.

Recommended filter device for short term use:

Use a respirator with multi-purpose combination (US) or type ABEK (EN 14387) as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards such as NIOSH (USA) or CEN (EU).

Protection of hands:

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

Penetration time of glove material (in minutes) Not determined

Eye protection: Safety glasses with side shields / NIOSH (US) or EN 166(EU)

Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General Information

Appearance:

Form:

Liquid

Odor:

Not determined

Odor threshold:

Not determined.

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Product name: 1,3,5-Trimethyl-1,4-cyclohexadiene

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pH-value:	Not determined.
Change in condition	
Melting point/Melting range:	Not determined
Boiling point/Boiling range:	172 °C (342 °F)
Sublimation temperature / start:	Not determined
Flash point:	35 °C (95 °F)
Flammability (solid, gaseous)	Not determined.
Ignition temperature:	Not determined
Decomposition temperature:	Not determined
Auto igniting:	Not determined.
Danger of explosion:	Product is not explosive. However, formation of explosive air/vapor mixtures is possible.
Explosion limits:	
Lower:	Not determined
Upper:	Not determined
Vapor pressure:	Not determined
Density at 20 °C (68 °F):	0.82 g/cm³ (6.843 lbs/gal)
Relative density	Not determined.
Vapor density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water:	Not miscible or difficult to mix
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not determined.
kinematic:	Not determined.
Other information	No further relevant information available.

10 Stability and reactivity

Reactivity No information known.

Chemical stability Stable under recommended storage conditions.

Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.

Possibility of hazardous reactions Reacts with strong oxidizing agents

Conditions to avoid No further relevant information available.

Incompatible materials: Oxidizing agents

Hazardous decomposition products: Carbon monoxide and carbon dioxide

11 Toxicological information

Information on toxicological effects

Acute toxicity: No effects known.

LD/LC50 values that are relevant for classification: No data

Skin irritation or corrosion: May cause irritation

Eye irritation or corrosion: May cause irritation

Sensitization: No sensitizing effects known.

Germ cell mutagenicity: No effects known.

Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.

Reproductive toxicity: No effects known.

Specific target organ system toxicity - repeated exposure: No effects known.

Specific target organ system toxicity - single exposure: No effects known.

Aspiration hazard: No effects known.

Subacute to chronic toxicity: No effects known.

Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity

Aquatic toxicity: No further relevant information available.

Persistence and degradability No further relevant information available.

Bioaccumulative potential No further relevant information available.

Mobility in soil No further relevant information available.

Additional ecological information:

General notes:

Do not allow material to be released to the environment without proper governmental permits.

Avoid transfer into the environment.

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods

Recommendation Consult state, local or national regulations to ensure proper disposal.

Uncleaned packagings:

Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number	
DOT, IMDG, IATA	UN3295
UN proper shipping name	
DOT	Hydrocarbons, liquid, n.o.s.
ADR	3295 Hydrocarbons, liquid, n.o.s.
IMDG, IATA	HYDROCARBONS, LIQUID, N.O.S.

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Product name: 1,3,5-Trimethyl-1,4-cyclohexadiene

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Transport hazard class(es) DOT 	
Class Label ADR	3 Flammable liquids 3
	
Class Label IMDG, IATA	3 (F1) Flammable liquids 3
	
Class Label	3 Flammable liquids 3
Packing group DOT, ADR, IMDG, IATA	III
Environmental hazards:	Not applicable.
Special precautions for user	Warning: Flammable liquids
EMS Number:	F-E,S-D
Stowage Category	A
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code Not applicable.	
Transport/Additional information:	
DOT	
Quantity limitations	On passenger aircraft/rail: 60 L On cargo aircraft only: 220 L
Marine Pollutant (DOT):	No
IMDG	
Limited quantities (LQ)	5L
Excepted quantities (EQ)	Code: E1 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 1000 ml
UN "Model Regulation":	UN 3295 HYDROCARBONS, LIQUID, N.O.S., 3, III

15 Regulatory information	
Safety, health and environmental regulations/legislation specific for the substance or mixture	
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)	
Hazard pictograms	
	
GHS02	
Signal word Warning	
Hazard statements	
H226 Flammable liquid and vapor.	
Precautionary statements	
P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.	
P280 Wear protective gloves / eye protection / face protection.	
P240 Ground/bond container and receiving equipment.	
P241 Use explosion-proof electrical/ventilating/lighting/equipment.	
P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.	
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.	
National regulations	
This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.	
This product is not listed on the Canadian Domestic Substances List (DSL) or the Canadian Non-Domestic Substances List (NDSL).	
SARA Section 313 (specific toxic chemical listings) Substance is not listed.	
California Proposition 65	
Prop 65 - Chemicals known to cause cancer Substance is not listed.	
Prop 65 - Developmental toxicity Substance is not listed.	
Prop 65 - Developmental toxicity, female Substance is not listed.	
Prop 65 - Developmental toxicity, male Substance is not listed.	
Information about limitation of use: For use only by technically qualified individuals.	
Other regulations, limitations and prohibitive regulations	
Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.	
The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.	
Substance is not listed.	
Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.	
Chemical safety assessment: A Chemical Safety Assessment has not been carried out.	

16 Other information	
Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.	
Department issuing SDS: Global Marketing Department	

Product name: 1,3,5-Trimethyl-1,4-cyclohexadiene

Date of preparation/Revision: Print date, revision date and version number are in the header of each page.

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Abbreviations and acronyms:

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
IATA-DSR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)
ICAO: International Civil Aviation Organisation
ICAO-TI: Technical Instructions by the "International Civil Aviation Organisation" (ICAO)
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
PBT: Persistent, Bioaccumulative and Toxic
SVHC: Substances of Very High Concern
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)
Flam. Liq. 3: Flammable liquids – Category 3