

SAFETY DATA SHEET

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

1.1 Product identifiers

Product name	2,2,4-Trimethylpentane
CAS number	540-84-1
Synonyms	Isooctane, Trimethylpentane

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

Identified uses	Laboratory Chemicals
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1.3 Details of the supplier of the safety data sheet

Company	Lab Alley, LLC 12501 Pauls Valley Road Austin, Texas 78737 U.S.A.
Telephone	512-668-9918
Fax	512-886-4008

1.4 Emergency telephone

Emergency Phone #	US & Canada: 1-800-535-5053	INFOTRAC
	International 1-352-323-3500	INFOTRAC


SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids Category 2
Skin Corrosion/irritation Category 2
Serious Eye Damage/Eye Irritation Category 2
Specific target organ toxicity (single exposure) Category 3
Target Organs - Central nervous system (CNS).
Aspiration Toxicity Category 1

2.2 GHS Label elements, including precautionary statements

Pictogram	
Signal Word	Danger
Hazard statements	Highly flammable liquid and vapor. May be fatal if swallowed and enters airways. Causes skin irritation. Causes serious eye irritation. May cause drowsiness or dizziness.

Precautionary statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling.
Wear protective gloves/protective clothing/eye protection/face protection.
Do not breathe dust/fume/gas/mist/vapors/spray.
Use only outdoors or in a well-ventilated area.
Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
Keep container tightly closed.
Ground/bond container and receiving equipment.
Use explosion-proof electrical/ventilating/lighting/equipment.
Use only non-sparking tools.
Take precautionary measures against static discharge.
Keep cool.

Response

Get medical attention/advice if you feel unwell.

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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

Skin

If skin irritation occurs: Get medical advice/attention.

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

Wash contaminated clothing before reuse.

Eyes

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.

Ingestion

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
Do NOT induce vomiting.

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction.

Storage

Store locked up.

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

Disposal

Dispose of contents/container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Very toxic to aquatic life with long lasting effects.

SECTION 3: Composition/information on ingredients

3.1 Components

Chemical name	Common name and synonyms	CAS number	Concentration
Isooctane	Trimethylpentane	540-84-1	>95

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice	If symptoms persist, call a physician.
If inhaled	Move to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs.
In case of skin contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
In case of eye contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Obtain medical attention.
If swallowed	Clean mouth with water and drink afterwards plenty of water. Do not induce vomiting. Call a physician or Poison Control Center immediately. If vomiting occurs naturally, have victim lean forward.

4.2 Most important symptoms and effects, both acute and delayed

None reasonably foreseeable. Inhalation of high vapor concentrations may cause symptoms like

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray.

Unsuitable extinguishing media Water may be ineffective, Do not use a solid water stream as it may scatter and spread fire.

5.2 Specific hazards arising from the substance or mixture

Flammable. Risk of ignition. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air. Do not allow run-off from fire fighting to enter drains or water courses.

5.3 Special protective equipment and precautions for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

5.4 Further information

Flash Point -12 °C / 10.4 °F

Autoignition Temperature 410 °C / 770 °F

Explosion limits

Upper 6.0 vol %

Lower 1.1 vol %

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge No information available

NFPA

Health	Flammability	Instability	Physical hazards
3	3	0	N/A

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

6.2 Environmental precautions

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

6.4 Reference to other sections

Refer to protective measures listed in Sections 7 and 8. See section 13 for proper disposal.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Wear personal protective equipment. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep away from open flames, hot surfaces and sources of ignition. Keep containers tightly closed in a dry, cool and well-ventilated place. Flammables area. Keep away from heat and sources of ignition.

Incompatibilities

Strong oxidizing agents, Strong acids, Strong bases.

SECTION 8: Exposure controls/personal protection

8.1 Occupational exposure limits

US. OSHA Table Z-1 Limits for Air Contaminants (29 CFR 1910.1000)

Component	Type	Value
Isooctane	-	-

US. ACGIH Threshold Limit Values

Component	Type	Value
Isooctane	TWA	300 ppm

US. NIOSH: Pocket Guide to Chemical Hazards

Component	Type	Value
Isooctane	-	-

Biological occupational exposure limits

No information available.

8.2 Exposure controls

Appropriate engineering controls

Use only under a chemical fume hood. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

Personal protective equipment

Eye/face protection

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin protection

Long sleeved clothing.

Body Protection

Long sleeved clothing.

Respiratory protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Control of environmental exposure

Handle in accordance with good industrial hygiene and safety practice.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	Petroleum distillates
Odor Threshold	No additional information
pH	No additional information
Melting Point/Range	-107 °C / -160.6 °F
Boiling Point/Range	98 - 99 °C / 208.4 - 210.2 °F @ 760 mmHg
Evaporation Rate	No additional information
Flammability (solid)	No additional information
Flammability or explosive limit	
Upper	6.0 vol %
Lower	1.1 vol %
Vapor Pressure	51 mbar @ 20 °C
Vapor Density	3.94
Specific Gravity	0.690
Solubility	Immiscible
Partition coefficient; n-octanol/water	No additional information
Autoignition Temp	410 °C / 770 °F
Decomposition Temp	No additional information
Viscosity	0.51 mPa s at 22 °C
Molecular Formula	C8 H18
Molecular Weight	114.23
VOC Content(%)	No additional information
Oxidizing properties	No additional information

9.2 Other safety information

No information available.

SECTION 10: Stability and reactivity

10.1 Reactivity

None known, based on information available.

10.2 Chemical stability

Stable under normal conditions.

10.3 Possibility of hazardous reactions

None under normal processing.

10.4 Conditions to avoid

Incompatible products. Heat, flames and sparks. Keep away from open flames, hot surfaces and sources of ignition.

10.5 Incompatible materials

Strong oxidizing agents, Strong acids, Strong bases.

10.6 Hazardous decomposition products

Carbon monoxide (CO), Carbon dioxide (CO₂).

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Product Information, Component Information

Acute toxicity

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isooctane	5000 mg/kg (Rat)	2000 mg/kg (Rabbit)	33.52 mg/L (Rat) 4 h

Skin corrosion/irritation

Irritating to eyes, respiratory system and skin.

Serious eye damage/eye irritation

Irritating to eyes, respiratory system and skin.

Respiratory or skin sensitization

No information available.

Germ cell mutagenicity

No information available.

Carcinogenicity

Component	CAS	IARC	NTP	ACGIH	OSHA	Mexico
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Isooctane	540-84-1	Not listed	Not listed	Not listed	Not listed	Not listed
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Specific target organ toxicity - single exposure

Central nervous system (CNS).

Specific target organ toxicity - repeated exposure

None known.

Reproductive toxicity

No information available.

Chronic effects

No information available.

11.2 Additional Information

The toxicological properties have not been fully investigated.

SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater	Freshwater Fish	Microtox	Water Flea
Isooctane	EC50= 2.94 mg/l, 72h	LC50 = 0.11 mg/l, 96h,(Rainbow trout)	Not listed	EC50= 0.4 mg/l, 48h (Daphnia magna)

12.2 Persistence and degradability

Insoluble in water. Persistence is unlikely based on information available. Immiscible with water.

12.3 Bio accumulative potential

No information available.

12.4 Mobility in soil

Will likely be mobile in the environment due to its volatility. Is not likely mobile in the environment due its low water solubility.

12.5 Results of PBT and vPvB assessment

No information available.

12.6 Endocrine disrupting properties

No information available.

12.7 Other adverse effects

No information available.

SECTION 13: Disposal considerations

13.1 Waste Disposal Methods

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

SECTION 14: Transport information

DOT (US)

UN Number	UN1262
Proper Shipping name	OCTANES
Hazard Class	3
Packaging Group	II

IMDG

UN Number	UN1262
Proper Shipping name	OCTANES
Hazard Class	3
Packaging Group	II

IATA

UN Number	UN1262
Proper Shipping name	OCTANES
Hazard Class	3
Packaging Group	II

SECTION 15: Regulatory information

US federal regulations

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not listed/applicable.

CERCLA Hazardous Substance List (40 CFR 302.4)

Isooctane: 1000 lb RQ.

SARA 304 Emergency release notification

Not listed/applicable.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not listed/applicable.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

SARA 302 Extremely hazardous substance

Not listed/applicable.

SARA 311/312 Hazardous

Acute Health Hazard: Yes

Chronic Health Hazard: Yes

Fire Hazard: Yes

SARA 313 (TRI reporting)

Not listed/applicable.

Other federal regulations

Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List

Isooctane: Listed.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not listed/applicable.

Safe Drinking Water Act

Not listed/applicable.

FEMA Priority Substances Respiratory Health and Safety in the Flavor Manufacturing Workplace

Not listed/applicable.

US state regulations

US. Massachusetts RTK - Substance List

Isooctane: Listed.

US. New Jersey Worker and Community Right-to-Know Act

Isooctane: Listed.

US. Pennsylvania Worker and Community Right-to-Know Law

Isooctane: Listed.

California Proposition 65

Not listed/applicable.

SECTION 16: Other information

Date of Issue: 6/24/2025

SECTION 17: Disclaimer

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.