

Classified as hazardous in accordance with the criteria of EPA New Zealand

Section 1 - Identification

Product Identifier

Product Name	<u>2,2,4-Trimethylpentane</u>
CAS No	540-84-1
Synonyms	Isooctane
Molecular Formula	C ₈ H ₁₈
Molecular Weight	114.23
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

Product Code 421980000; 421980025; 421980040; 421985000

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Section 2 - Hazard(s) Identification

Classification under Work Safe New Zealand

Classified as hazardous in accordance with the criteria of EPA New Zealand

HSNO Approval Number HSR001176

GHS Classification

Physical hazards

Flammable liquids

Category 2

Health hazards

Aspiration Toxicity

Category 1

Skin Corrosion/Irritation

Category 2

Serious Eye Damage/Eye Irritation

Category 2

Specific target organ toxicity - (single exposure)

Category 3

Environmental hazards

Acute aquatic toxicity

Category 1

Chronic aquatic toxicity

Category 1

Label Elements**Signal Word****Danger****Hazard Statements**

H225 - Highly flammable liquid and vapor
 H304 - May be fatal if swallowed and enters airways
 H315 - Causes skin irritation
 H336 - May cause drowsiness or dizziness
 H410 - Very toxic to aquatic life with long lasting effects
 H319 - Causes serious eye irritation

Precautionary Statements**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
 P264 - Wash face, hands and any exposed skin thoroughly after handling
 P271 - Use only outdoors or in a well-ventilated area
 P280 - Wear protective gloves/protective clothing/eye protection/face protection
 P273 - Avoid release to the environment

Response

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor
 P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
 P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
 P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
 P312 - Call a POISON CENTER or doctor if you feel unwell
 P331 - Do NOT induce vomiting
 P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
 P362 + P364 - Take off contaminated clothing and wash it before reuse
 P391 - Collect spillage

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Other hazards which do not result in classification

Section 3 - Composition and Information on Ingredients

Component	CAS No	Weight %
Isooctane	540-84-1	>95

Section 4 - First Aid Measures

Description of first aid measures

General Advice	If symptoms persist, call a physician.
New Zealand Emergency Tel.	CHEMTREC® 09 980 6780 or +64 9 980 6780
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs (by aspiration).
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Ingestion	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.
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.
First Aid Facilities	Eyewash, safety shower and washroom.
Most important symptoms and effects	None reasonably foreseeable. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically. Symptoms may be delayed.

Section 5 - Fire Fighting Measures

Suitable Extinguishing Media

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

Do not use a solid water stream as it may scatter and spread fire.

Specific Hazards Arising from the Chemical

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.

Hazardous Combustion Products

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

Special protective equipment and precautions for fire fighters

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

Section 6 - Accidental Release Measures

Personal Precautions, Protective Equipment and Emergency Procedures

Emergency procedures

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

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.

Methods for Containment and Clean 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.

Precautions to prevent secondary hazards

Clean contaminated objects and areas thoroughly observing environmental regulations

Reference to Other Sections

Refer to protective measures listed in Sections 8 and 13.

Section 7 - Handling and Storage

Precautions for Safe Handling**Advice on safe handling**

Wear personal protective equipment/face protection. 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. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

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, sparks and flame.

Incompatible Materials

Strong oxidizing agents. Strong acids. Strong bases.

AS/NZS 2243.10:2004, Safety in laboratories - Storage of chemicals

AS 1940-2004 - The storage and handling of flammable and combustible liquids

Section 8 - Exposure Controls and Personal Protection

Control parameters**Exposure limits**

ACGIH - Threshold Limit Values - Ceiling (TLV-C) guidelines by the American Conference of Governmental Industrial Hygienists (ACGIH) for controlling worker exposure to airborne chemical concentrations in the workplace.

Component	New Zealand WEL	Australia	ACGIH TLV	The United Kingdom
Isooctane			TWA: 300 ppm	

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Appropriate engineering controls**Engineering Measures**

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. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment

changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Individual protection measures, such as personal protective equipment

Eye Protection Wear safety glasses with side shields (or goggles) (Australian/New Zealand Standard AS/NZS 1337 - Eye protectors for Industrial applications)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	AUS/NZ Standard	Glove comments
Nitrile rubber, Viton (R),	> 480 minutes	0.3 mm	AS/NZS 2161	As tested under EN374-3 Determination of Resistance to Permeation by Chemicals
Neoprene, Natural rubber, PVC.	> 480 minutes	0.35 mm		
Neoprene gloves	> 480 minutes	0.45 mm		

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection Long sleeved clothing

Respiratory Protection Use an AS/NZS 1716 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained in line with AS/NZS 1715 on the use and maintenance of respiratory protective devices

Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN371 (or AUS/NZ equivalent)

Recommended half mask:- Valve filtering: EN405 or Half mask: EN140 plus filter, EN 371 (or AUS/NZ equivalent)

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls Prevent product from entering drains. Do not allow material to contaminate ground water system. Local authorities should be advised if significant spillages cannot be contained.

Section 9 - Physical and Chemical Properties

Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Colorless	
Odor	Petroleum distillates	
Odor Threshold	No data available	
pH	Not applicable	
Melting Point/Range	-107 °C / -160.6 °F	
Softening Point	No data available	
Boiling Point/Range	98 - 99 °C / 208.4 - 210.2 °F	@ 760 mmHg
Flammability (liquid)	Highly flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 1.1 vol % Upper 6 vol %	
Flash Point	-12 °C / 10.4 °F	Method - No information available
Autoignition Temperature	410 °C / 770 °F	
Decomposition Temperature	No data available	
Viscosity	0.51 mPa s at 22 °C	
Water Solubility	Immiscible	
Solubility in other solvents	No information available	

Partition Coefficient (n-octanol/water)

Vapor Pressure	51 mbar @ 20 °C	
Density / Specific Gravity	0.690	
Bulk Density	Not applicable	Liquid
Vapor Density	3.94	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

Other information

Molecular Formula	C8 H18
Molecular Weight	114.23
Explosive Properties	Vapors may form explosive mixtures with air

Section 10 - Stability and Reactivity

Reactivity	None known, based on information available
Stability	Stable under normal conditions.
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.
Conditions to Avoid	Incompatible products, Heat, flames and sparks, Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Strong oxidizing agents, Strong acids, Strong bases.
Hazardous Decomposition Products	Carbon monoxide (CO). Carbon dioxide (CO ₂).

Section 11 - Toxicological Information

Acute Effects**Information on likely routes of exposure****Product Information**

Inhalation	Irritating to respiratory system. May be harmful if inhaled. INHALATION MAY CAUSE CENTRAL NERVOUS SYSTEM EFFECTS.
Eyes	Irritating to eyes.
Skin	Irritating to skin. May be harmful in contact with skin.
Ingestion	May be harmful if swallowed. Aspiration hazard. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea. Harmful if swallowed. Potential for aspiration if swallowed.

Numerical measures of toxicity**(a) acute toxicity;**

Oral	Based on available data, the classification criteria are not met
Dermal	Based on available data, the classification criteria are not met
Inhalation	Based on available data, the classification criteria are not met

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

(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Based on available data, the classification criteria are not met
(d) respiratory or skin sensitization;	
Respiratory	Based on available data, the classification criteria are not met
Skin	Based on available data, the classification criteria are not met
(e) germ cell mutagenicity;	Based on available data, the classification criteria are not met
(f) carcinogenicity;	Based on available data, the classification criteria are not met There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	Based on available data, the classification criteria are not met
(h) STOT-single exposure;	Category 3
Effective dose	NOAEL 2220 ppm 6hr/day
Results / Target organs	Central nervous system (CNS)
(i) STOT-repeated exposure;	Based on available data, the classification criteria are not met
Target Organs	None known.
(j) aspiration hazard;	Category 1
Other Adverse Effects	The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed

Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

Section 12 - Ecological Information

Ecotoxicity

Aquatic ecotoxicity

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 Fish	Water Flea	Freshwater Algae	Microtox
Isooctane	LC50 = 0.11 mg/l, 96h, (Rainbow trout)	EC50 = 0.4 mg/l, 48h (Daphnia magna)	EC50 = 2.94 mg/l, 72h	

Terrestrial ecotoxicity

There is no data for this product

Persistence and Degradability**Persistence**

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

Degradation in sewage treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Bioaccumulative Potential	May have some potential to bioaccumulate
Bioconcentration factor (BCF)	231
Mobility	Spillage unlikely to penetrate soil. The product is insoluble and floats on water. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Is not likely mobile in the environment due its low water solubility.
<u>Other adverse effects</u>	
Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance

Section 13 - Disposal Considerations

Waste treatment methods

Waste from Residues/Unused Products	Do not allow into drains or watercourses or dispose of where ground or surface waters may be affected. Wastes, including emptied containers, are controlled wastes and should be disposed of in accordance with all federal, E.P.A., state and local regulations. Assure conformity with all applicable regulations.
Contaminated Packaging	Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.
Other Information	Disposal agencies or waste contractors must comply with the New Zealand Hazardous Substances (Disposal) Regulations . Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Can be landfilled or incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains.

Section 14 - Transport Information

NZS 5433:2020

UN-No	UN1262
Proper Shipping Name	OCTANES
Hazard Class	3
Packing Group	II

IATA

UN-No	UN1262
Proper Shipping Name	OCTANES
Hazard Class	3
Packing Group	II

IMDG/IMO

UN-No	UN1262
Proper Shipping Name	OCTANES
Hazard Class	3
Packing Group	II

Component	IMDG Marine Pollutant
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Isooctane 540-84-1 (>95)	IMDG regulated marine pollutant (Listed in the index) IMDG regulated marine pollutant (UN1262)
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Environmental hazards	Dangerous for the environment Product is a marine pollutant according to the criteria set by IMDG/IMO
Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	Not applicable, packaged goods
Special Precautions	No special precautions required. Please refer to the applicable dangerous goods regulations for additional information.
Additional information	None known

Section 15 - Regulatory Information

Safety, health and environmental regulations/legislation specific for the substance or mixture

HSNO Approval Number	HSR001176
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National Regulations

There are no applicable tolerable exposure limits or environmental exposure limits according to the EPA Controls for Hazardous Substances

Certified handlers, tracking and controlled substance license requirements

Certified handlers are required for some substances. This includes substances requiring a controlled substance license, and most explosives, vertebrates toxic agents, and certain fumigants. Acutely toxic substances which are a Category 1 or 2, such as pesticides also require Certified handlers. Please check the Health and Safety at Work Act 2015 for further information. Tracking is required for some highly hazardous substances. These substances need to be under the control of an appropriately trained person or appropriately secured. Please check the Health and Safety at Work Act 2015 for further information.

Prohibition or notification/licensing requirements

Shown below are details of specific prohibition/notifications or licencing requirements when they apply.

International Regulations

Ozone Depletion Potential This product does not contain any known or suspected substance

Persistent Organic Pollutant This product does not contain any known or suspected substance

Rotterdam Convention (PIC) Not applicable

Component	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	IMDG Marine Pollutant
Isooctane			IMDG regulated marine pollutant (Listed in the index) IMDG regulated marine pollutant (UN1262)

Authorisation/Restrictions according to EU REACH

Component	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Isooctane	-	Use restricted. See item 75. (see link for restriction details)	-

<https://echa.europa.eu/substances-restricted-under-reach>

International Inventories

New Zealand (NZIoC), Australia (AICS), Europe (EINECS/ELINCS/NLP), Korea (KECL), China (IECSC), Taiwan (TCSI), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	NZIoC	AICS	EINECS	ELINCS	NLP	KECL	IECSC	TCSI
Isooctane	540-84-1	X	X	208-759-1	-	-	KE-34634	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	PICCS	ISHL	ENCS
Isooctane	540-84-1	X	ACTIVE	X	-	X	X	X

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Section 16 - Other Information

This safety data sheet complies with the requirements of the EPA Hazardous Substances (Hazard Classification) Notice 2020 and WorkSafe New Zealand Regulations

Legend

NZIoC - New Zealand Inventory of Chemicals

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

IECSC - Chinese Inventory of Existing Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

NZS 5433:2020 - Transport of Dangerous Goods on Land

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

WEL - Workplace Exposure Limit

DNEL - Derived No Effect Level

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

VOC - (Volatile Organic Compound)

AICS - Australian Inventory of Chemical Substances

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

CAS - Chemical Abstracts Service

ACGIH - American Conference of Governmental Industrial Hygienists

PNEC - Predicted No Effect Concentration

OECD - Organisation for Economic Co-operation and Development

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

ADG - Australian Code for the Transport of Dangerous Goods by Road and Rail

LC50 - Lethal Concentration 50%

ATE - Acute Toxicity Estimate

RPE - Respiratory Protective Equipment

NOEC - No Observed Effect Concentration

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PBT - Persistent, Bioaccumulative, Toxic

Key literature references and sources for data

HSNO classifications provided in the New Zealand Chemical Classification Information Database (CCID).

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

EPA Guide to classifying hazardous substances in New Zealand

EPA - Assigning a product to an existing HSNO approval guide

Training Advice

Chemical incident response training.

Revision Date

10-Mar-2023

Revision Summary

Not applicable

Disclaimer

The information provided in 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 guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered 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 materials or in any process, unless specified in the text

End of Safety Data Sheet