ALFAAC29572

2,2,4-Trimethylpentane

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: **2,2,4-Trimethylpentane**
Product Description: **2,2,4-Trimethylpentane**

Cat No. : **C29572**
Synonyms Isooctane
CAS No 540-84-1
Molecular Formula C8 H18

Supplier

Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
Shore Road, Heysham
Lancashire, LA3 2XY,
United Kingdom
Office Tel: +44 (0) 1524 850506
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Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No. **US:**001-800-424-9300 / **Europe:**001-703-527-3887

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State	**Appearance**	**Odor**
Liquid	Colorless	Petroleum distillates

Emergency Overview

Highly flammable liquid and vapor. May be fatal if swallowed and enters airways. Causes skin irritation. May cause drowsiness and dizziness. Very toxic to aquatic life with long lasting effects. May be harmful if swallowed.

Classification of the substance or mixture

Flammable liquids.	Category 2
Aspiration Toxicity	Category 1
Acute Oral Toxicity	Category 5
Skin Corrosion/Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3
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
H303 - May be harmful if swallowed

Precautionary Statements
Prevention
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
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
P270 - Do not eat, drink or smoke when using this product
P271 - Use only outdoors or in a well-ventilated area
P280 - Wear protective gloves/protective clothing/eye protection/face protection
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
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

Physical and Chemical Hazards
Vapors may cause flash fire or explosion. Highly flammable.
Health Hazards
Aspiration hazard if swallowed - can enter lungs and cause damage. Causes skin irritation. May cause drowsiness or dizziness. May be harmful if swallowed.
Environmental hazards
Very toxic to aquatic life with long lasting effects. Will likely be mobile in the environment due to its volatility. Is not likely mobile in the environment due its low water solubility. 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.

Other Hazards

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

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

SECTION 4. FIRST AID MEASURES

General Advice
If symptoms persist, call a physician.

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.

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).

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.

Most important symptoms and effects
None reasonably foreseeable. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

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.

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.

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal Precautions
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.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

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.

Storage
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.

Specific Use(s)
Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

Component	China	Taiwan	Thailand	Hong Kong
Isooctane	-	-		STEL: 375 ppm STEL: 1750 mg/m³

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
Isooctane	TWA: 300 ppm			-	

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

Monitoring methods
BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure 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.

Personal protective equipment

Eye Protection Wear safety glasses with side shields (or goggles) (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	> 480 minutes		Level 6	As tested under EN374-3 Determination of
Viton (R)	> 480 minutes		EN 374	Resistance to Permeation by Chemicals

Neoprene		0.3 mm
Natural rubber		0.35 mm
PVC		
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 compatability, 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 When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN371

Small scale/Laboratory use Maintain adequate ventilation Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 371

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

Appearance	Colorless	
Physical State	Liquid	
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
Flash Point	-12 °C / 10.4 °F	**Method -** No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	**Lower** 1.1 vol % **Upper** 6 vol %	
Vapor Pressure	51 mbar @ 20 °C	
Vapor Density	3.94	(Air = 1.0)
Specific Gravity / Density	0.690	
Bulk Density	Not applicable	Liquid
Water Solubility	Immiscible	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	410 °C / 770 °F	
Decomposition Temperature	No data available	
Viscosity	0.51 mPa s at 22 °C	

Explosive Properties	Vapors may form explosive mixtures with air
Oxidizing Properties	No information available
Molecular Formula	C8 H18
Molecular Weight	114.23

SECTION 10. STABILITY AND REACTIVITY

Stability Stable under normal conditions.

Hazardous Reactions None under normal processing.

Hazardous Polymerization Hazardous polymerization does not occur.

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

Materials to avoid Strong oxidizing agents. Strong acids. Strong bases.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO_2).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

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 effects 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	

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 in soil 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

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 from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local 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 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

Road and Rail Transport

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

IATA

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

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION

International Inventories
X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Isooctane	X	X	X	X	208-759-1	X	X	X	X	X	X	KE-34634

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Creation Date 22-Jun-2009
Revision Date 13-May-2024
Revision Summary New emergency telephone response service provider.

Training Advice
Chemical incident response training.

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances
PICCS - Philippines Inventory of Chemicals and Chemical Substances
IECSC - Chinese Inventory of Existing Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances

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

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List
ENCS - Japanese Existing and New Chemical Substances
AICS - Australian Inventory of Chemical Substances
NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit
ACGIH - American Conference of Governmental Industrial Hygienists
DNEL - Derived No Effect Level
RPE - Respiratory Protective Equipment
LC50 - Lethal Concentration 50%
NOEC - No Observed Effect Concentration
PBT - Persistent, Bioaccumulative, Toxic
TWA - Time Weighted Average
IARC - International Agency for Research on Cancer
PNEC - Predicted No Effect Concentration
LD50 - Lethal Dose 50%
EC50 - Effective Concentration 50%
POW - Partition coefficient Octanol:Water
vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road
OECD - Organisation for Economic Co-operation and Development 231
IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code
MARPOL - International Convention for the Prevention of Pollution from Ships
ATE - Acute Toxicity Estimate
VOC - (Volatile Organic Compound)

Key literature references and sources for data
https://echa.europa.eu/information-on-chemicals
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

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End of Safety Data Sheet