

ACR32694

2,2,4-Trimethylpentane

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

产品说明: 2,2,4-三甲基戊烷
Product Description: 2,2,4-Trimethylpentane

Cat No. : 326940000; 326940010; 326941000
Synonyms Isooctane
CAS No 540-84-1
Molecular Formula C8 H18

Supplier

UK entity/business name
Fisher Scientific UK
Bishop Meadow Road,
Loughborough, Leicestershire LE11 5RG, United Kingdom
General info; Tel: +44 (0)1509 231166

EU entity/business name
Acros Organics BVBA
Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium
General Info; Tel: +32-14-57 52 11 (info@acros.com)
Technical Support; Tel +32-14-56 56 00 (acros.techsupport@thermofisher.com)

Emergency Telephone Number For information **US** call: 001-800-ACROS-01 / **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
Liquid

Appearance
Colorless

Odor
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

2,2,4-Trimethylpentane

**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/sparks/open flames/hot surfaces. - No smoking
 P240 - Ground/bond container and receiving equipment
 P241 - Use explosion-proof electrical/ ventilating/ lighting equipment
 P242 - Use non-sparking tools
 P243 - Take precautionary measures against static discharge
 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/physician
 P303 + P361 + P353 - IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/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
 P363 - Wash contaminated clothing before reuse
 P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction

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**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	Hong Kong	The United Kingdom
Isooctane	-	-	STEL: 375 ppm STEL: 1750 mg/m ³	-

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	European Union
Isooctane	TWA: 300 ppm			

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 Resistance to Permeation by Chemicals
Viton (R)	> 480 minutes		EN 374	
Neoprene				
Natural rubber				

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PVC	0.3 mm
	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 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

SAFETY DATA SHEET

2,2,4-Trimethylpentane

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 (CO₂).

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.

SAFETY DATA SHEET

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(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
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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
Persistent Organic Pollutant
Ozone Depletion Potential

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

2,2,4-Trimethylpentane

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**

Creation Date 22-Jun-2009
Revision Date 18-Dec-2020
Revision Summary Not applicable.

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

2,2,4-Trimethylpentane**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
Predicted No Effect Concentration (PNEC)**LD50** - Lethal Dose 50%**EC50** - Effective Concentration 50%**POW** - Partition coefficient Octanol:Water**vPvB** - very Persistent, very Bioaccumulative**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code**OECD** - Organisation for Economic Co-operation and Development
231**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association**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

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