

Creation Date Oct-2013

Revision Date Oct-2018

Revision Number 2

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identification

**Product Description:** 2,2,4-Trimethylpentane  
**Product Grade:** SQ, ER, HPLC  
**Cat No. :** Q43596, Q12705, Q12707, Q26175  
**Synonyms** Isooctane  
**CAS-No** 540-84-1  
**EC-No.** 208-759-1  
**Molecular Formula** C8 H18  
**Reach Registration Number** 01-2119457965-22

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

**Recommended Use** Laboratory chemicals.  
**Sector of use** SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites  
**Product category** PC21 - Laboratory chemicals  
**Process categories** PROC15 - Use as a laboratory reagent  
**Environmental release category** ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)  
**Uses advised against** No Information available

### 1.3. Details of the supplier of the safety data sheet

**Company** Thermo Fisher Scientific India Pvt. Ltd  
 403-404, B-wing, Delphi, Hiranandani Business Park,  
 Powai, Mumbai 400076, INDIA.  
**E-mail address** [laboratorysolutions@thermofisher.com](mailto:laboratorysolutions@thermofisher.com)

### 1.4. Emergency telephone number

India Toll Free: 18 00 22 22 30  
 Chemtrec US: (800)424-9300  
 Chemtrec EU: 001(202)483-7616

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - Regulation (EC) No 1272/2008

##### Physical hazards

Flammable liquids Category 2 (H225)

##### Health hazards

Aspiration Toxicity Category 1 (H304)  
 Skin Corrosion/irritation Category 2 (H315)  
 Specific target organ toxicity - (single exposure) Category 3 (H336)

##### Environmental hazards

Acute aquatic toxicity Category 1 (H400)  
 Chronic aquatic toxicity Category 1 (H410)

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## 2.2. 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

### Precautionary Statements

- P210 - Keep away from heat/sparks/open flames/hot surfaces. - No smoking
- P303 + P361 + P353 - IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower
- P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician
- P331 - Do NOT induce vomiting
- P280 - Wear protective gloves/ protective clothing
- P304 + P340 - IF INHALED: Remove to fresh air and keep at rest in a position comfortable for breathing

## 2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008
Isooctane	540-84-1	EEC No. 208-759-1	>95	Skin Irrit. 2 (H315) STOT SE 3 (H336) Asp. Tox. 1 (H304) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410) Flam. Liq. 2 (H225)

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Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of 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. Obtain medical attention.

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<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
<b>Ingestion</b>	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.
<b>Inhalation</b>	Move to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs.
<b>Protection of First-aiders</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

#### **4.2. Most important symptoms and effects, both acute and delayed**

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

#### **4.3. Indication of any immediate medical attention and special treatment needed**

**Notes to Physician** Treat symptomatically. Symptoms may be delayed.

## **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.

##### **Extinguishing media which must not be used for safety reasons**

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

#### **5.2. Special 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.

##### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

#### **5.3. Advice 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**

#### **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 material for containment and cleaning up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use

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spark-proof tools and explosion-proof equipment.

## 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## 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. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing before re-use. Wash hands before breaks and at the end of workday.

### 7.2. Conditions for safe storage, including any incompatibilities

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.

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### Exposure limits

List source(s):

Component	European Union	The United Kingdom	France	Belgium	Spain
Isooctane			TWA / VME: 1000 mg/m <sup>3</sup> (8 heures). STEL / VLCT: 1500 mg/m <sup>3</sup> .		TWA / VLA-ED: 300 ppm (8 horas) TWA / VLA-ED: 1420 mg/m <sup>3</sup> (8 horas)

  

Component	Italy	Germany	Portugal	The Netherlands	Finland
Isooctane			TWA: 300 ppm 8 horas		TWA: 300 ppm 8 tunteina TWA: 1400 mg/m <sup>3</sup> 8 tunteina STEL: 380 ppm 15 minuutteina STEL: 1800 mg/m <sup>3</sup> 15 minuutteina

  

Component	Austria	Denmark	Switzerland	Poland	Norway
Isooctane	MAK-KZW: 1200 ppm 15 Minuten MAK-KZW: 5600 mg/m <sup>3</sup> 15 Minuten MAK-TMW: 300 ppm 8 Stunden MAK-TMW: 1400 mg/m <sup>3</sup> 8 Stunden		STEL: 600 ppm 15 Minuten STEL: 2800 mg/m <sup>3</sup> 15 Minuten TWA: 300 ppm 8 Stunden TWA: 1400 mg/m <sup>3</sup> 8 Stunden		TWA: 40 ppm 8 timer TWA: 275 mg/m <sup>3</sup> 8 timer

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## Biological limit values

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

## 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

**Derived No Effect Level (DNEL)** No information available

<u>Route of exposure</u>	<b>Acute effects (local)</b>	<b>Acute effects (systemic)</b>	<b>Chronic effects (local)</b>	<b>Chronic effects (systemic)</b>
Oral				699 mg/kg bw/day
Dermal				773 mg/kg bw/day
Inhalation				2035 mg/m <sup>3</sup>

**Predicted No Effect Concentration (PNEC)** No information available.

## 8.2. 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

Safety glasses with side-shields (European standard - EN 166)

#### Hand Protection

Protective gloves

<b>Glove material</b>	<b>Breakthrough time</b>	<b>Glove thickness</b>	<b>EU standard</b>	<b>Glove comments</b>
Nitrile rubber	> 480 minutes	0.3 mm	Level 6	As tested under EN374-3 Determination of Resistance to Permeation by Chemicals
Viton (R)	> 480 minutes	0.35 mm	EN 374	
Neoprene				
Natural rubber				
PVC				
Neoprene gloves	> 480 minutes	0.45 mm		

#### Skin and body protection

Long sleeved clothing

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.

#### 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

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**Small scale/Laboratory use** Maintain adequate ventilation

**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

### 9.1. Information on basic physical and chemical properties

<b>Appearance</b>	Colorless	
<b>Physical State</b>	Liquid	
<b>Odor</b>	Petroleum distillates	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	Not applicable	
<b>Melting Point/Range</b>	-107 °C / -160.6 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	98 - 99 °C / 208.4 - 210.2 °F	@ 760 mmHg
<b>Flash Point</b>	-12 °C / 10.4 °F	<b>Method</b> - No information available
<b>Evaporation Rate</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	<b>Lower</b> 1.1 vol % <b>Upper</b> 6 vol %	
<b>Vapor Pressure</b>	51 mbar @ 20 °C	
<b>Vapor Density</b>	3.94	(Air = 1.0)
<b>Specific Gravity / Density</b>	0.690	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Water Solubility</b>	Immiscible	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Autoignition Temperature</b>	410 °C / 770 °F	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	0.51 mPa s at 22 °C	
<b>Explosive Properties</b>	No information available	Vapors may form explosive mixtures with air
<b>Oxidizing Properties</b>	No information available	

### 9.2. Other information

**Molecular Formula** C8 H18  
**Molecular Weight** 114.23

## 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

**Hazardous Polymerization** Hazardous polymerization does not occur.  
**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.

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## 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on toxicological effects

#### Product Information

#### (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

### 12.1. Toxicity

#### 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	

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## 12.2. 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.

## 12.3. Bioaccumulative potential Bioconcentration factor (BCF)

May have some potential to bioaccumulate  
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## 12.4. 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.

## 12.5. Results of PBT and vPvB assessment

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB).

## 12.6. Other adverse effects

### **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

### 13.1. Waste treatment methods

#### **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.

#### **European Waste Catalogue (EWC)**

According to the European Waste Catalogue, Waste Codes are not product specific, but application specific.

#### **Other Information**

Do not dispose of waste into sewer. Waste codes should be assigned by the user based on the application for which the product was used. Can be incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

#### 14.1. UN number

UN1262

#### 14.2. UN proper shipping name

OCTANES

#### 14.3. Transport hazard class(es)

3

#### 14.4. Packing group

II

### ADR

#### 14.1. UN number

UN1262

#### 14.2. UN proper shipping name

OCTANES

#### 14.3. Transport hazard class(es)

3

#### 14.4. Packing group

II

### IATA

#### 14.1. UN number

UN1262

#### 14.2. UN proper shipping name

OCTANES

#### 14.3. Transport hazard class(es)

3

FSUT3600



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**14.4. Packing group** II

**14.5. Environmental hazards** Dangerous for the environment  
Product is a marine pollutant according to the criteria set by IMDG/IMO

**14.6. Special precautions for user** No special precautions required

**14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

International Inventories X = listed

Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	IECSC	AICS	KECL
Isooctane	208-759-1	-		X	X	-	X	X	X	X	X

### National Regulations

**WGK Classification** Water contaminating class (Germany): Hazardous to water/Class 2

Component	Germany - Water Classification (VwVwS)	Germany - TA-Luft Class
Isooctane	WGK 2	

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment.

Take note of Dir 94/33/EC on the protection of young people at work

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work

### 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3

H304 - May be fatal if swallowed and enters airways

H315 - Causes skin irritation

H336 - May cause drowsiness or dizziness

H400 - Very toxic to aquatic life

H410 - Very toxic to aquatic life with long lasting effects

H225 - Highly flammable liquid and vapor

### 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

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**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

**Key literature references and sources for data**

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

**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 Compounds

**Training Advice**

Chemical incident response training.

**Creation Date** Oct-2013

**Next Revision Date** Oct-2023

**Revision Summary** SDS section 1 updated and update of Format.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006**

**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**