

Creation Date 22-Jun-2009

Revision Date 11-Dec-2020

Revision Number 11

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

**1.1. Product identifier**

Product Description: **2,2,4-Trimethylpentane**  
 Cat No. : **167910000; 167910025; 167915000**  
 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 **UK entity/business name**  
 Fisher Scientific UK  
 Bishop Meadow Road, Loughborough,  
 Leicestershire LE11 5RG, United Kingdom

**EU entity/business name**  
 Acros Organics BVBA  
 Janssen Pharmaceuticaaan 3a  
 2440 Geel, Belgium

E-mail address [bege.sdsdesk@thermofisher.com](mailto:bege.sdsdesk@thermofisher.com)

**1.4. 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

**SECTION 2: HAZARDS IDENTIFICATION**

**2.1. Classification of the substance or mixture**

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

**Physical hazards**

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Flammable liquids	Category 2 (H225)
<b>Health hazards</b>	
Aspiration Toxicity	Category 1 (H304)
Skin Corrosion/Irritation	Category 2 (H315)
Specific target organ toxicity - (single exposure)	Category 3 (H336)
<b>Environmental hazards</b>	
Acute aquatic toxicity	Category 1 (H400)
Chronic aquatic toxicity	Category 1 (H410)

Full text of Hazard Statements: see section 16

## 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

- 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 victim to fresh air and keep at rest in a position comfortable for breathing
- P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
- P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

## 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	Flam. Liq. 2 (H225)

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				Asp. Tox. 1 (H304) Skin Irrit. 2 (H315) STOT SE 3 (H336) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)
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Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Isooctane	-	1	-

<b>Reach Registration Number</b>	01-2119457965-22
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Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>General Advice</b>	If symptoms persist, call a physician.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<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>	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).
<b>Self-Protection of the First Aider</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**

Water spray, carbon dioxide (CO<sub>2</sub>), 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.

### 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.

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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 as required. 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 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/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.

### 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, sparks and flame.

**Technical Rules for Hazardous Substances (TRGS) 510 Storage Class (LGK)**  
(Germany)

Class 3

### 7.3. Specific end use(s)

Use in laboratories

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## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### Exposure limits

List source(s):

#### 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

Route of exposure	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
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** 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	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.

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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

**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

## 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

Physical State	Liquid	
Appearance	Colorless	
Odor	Petroleum distillates	
Odor Threshold	No data available	
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	<b>Lower</b> 1.1 vol % <b>Upper</b> 6 vol %	
Flash Point	-12 °C / 10.4 °F	<b>Method -</b> No information available
Autoignition Temperature	410 °C / 770 °F	
Decomposition Temperature	No data available	
pH	Not applicable	
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)	

### 9.2. Other information

Molecular Formula	C8 H18
Molecular Weight	114.23

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**Explosive Properties** Vapors may form explosive mixtures with air

## 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.

**10.6. Hazardous decomposition products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### 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

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- (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.

## 11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## 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
Isooctane	LC50 = 0.11 mg/l, 96h, (Rainbow trout)	EC50= 0.4 mg/l, 48h (Daphnia magna)	EC50= 2.94 mg/l, 72h

Component	Microtox	M-Factor
Isooctane		1

### 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

May have some potential to bioaccumulate

#### Bioconcentration factor (BCF)

231

### 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

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



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assessment and very bioaccumulative (vPvB).

## 12.6. Endocrine disrupting properties

**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors

## 12.7. Other adverse effects

**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

### 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 Catalog, Waste Codes are not product specific, but application specific.

**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

### 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  
**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. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

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## SECTION 15: REGULATORY INFORMATION

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

#### International Inventories

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

Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	IECSC	AICS	KECL
Isooctane	208-759-1	-		X	X	-	X	X	X	X	KE-3463 4

#### Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

#### National Regulations

#### WGK Classification

See table for values

Component	Germany - Water Classification (VwVwS)	Germany - TA-Luft Class
Isooctane	WGK2	

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

### 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

**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

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**PBT** - Persistent, Bioaccumulative, Toxic

**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

**Key literature references and sources for data**

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

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 compound)

**Training Advice**

Chemical incident response training.

**Creation Date** 22-Jun-2009

**Revision Date** 11-Dec-2020

**Revision Summary** Update to CLP Format.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006  
COMMISSION REGULATION (EU) 2020/878 amending Annex II to 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**