SAFETY DATA SHEET

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

Creation Date 22-Jun-2009 **Revision Date** 29-Sep-2023 **Revision Number** 12

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

1.1. Product identifier

Product Description:	**2,2,4-Trimethylpentane**
Cat No. :	**268810000; 268810010; 268810025**
Synonyms	Isooctane
Index No	601-009-00-8
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
Thermo Fisher Scientific
Janssen Pharmaceuticalaan 3a, 2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. 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

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

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)

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 person to fresh air and keep 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)

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to

				GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Isooctane	540-84-1	EEC No. 208-759-1	>95	Flam. Liq. 2 (H225) Asp. Tox. 1 (H304) Skin Irrit. 2 (H315) STOT SE 3 (H336) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)

Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Isooctane	-	1	-

REACH registration number	01-2119457965-22

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. 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.

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).

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.

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 (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.

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_2).

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

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

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)
See table for values

Component	Acute effects local (Oral)	Acute effects systemic (Oral)	Chronic effects local (Oral)	Chronic effects systemic (Oral)
Isooctane 540-84-1 (>95)				699 mg/kg bw/day

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
Isooctane 540-84-1 (>95)				DNEL = 773mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Isooctane 540-84-1 (>95)				DNEL = 2035mg/m³

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
Viton (R)	> 480 minutes	0.35 mm	EN 374	Resistance to Permeation by Chemicals
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 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.

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	**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	
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
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_2).

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

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

SECTION 15: REGULATORY INFORMATION

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

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

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

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
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)

Authorisation/Restrictions according to EU REACH

Component	CAS No	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	540-84-1	-	Use restricted. See item 75. (see link for restriction details)	-

REACH links
https://echa.europa.eu/substances-restricted-under-reach

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
Isooctane	540-84-1	Not applicable	Not applicable

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

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?
Not applicable

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 .

National Regulations

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

WGK Classification See table for values

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

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
Isooctane 540-84-1 (>95)	Prohibited and Restricted Substances		

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

TWA - Time Weighted Average
IARC - International Agency for Research on Cancer

DNEL - Derived No Effect Level
RPE - Respiratory Protective Equipment
LC50 - Lethal Concentration 50%
NOEC - No Observed Effect Concentration
PBT - Persistent, Bioaccumulative, Toxic
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
BCF - Bioconcentration factor
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

Training Advice
Chemical incident response training.

Creation Date	22-Jun-2009
Revision Date	29-Sep-2023
Revision Summary	Not applicable.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

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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