SAFETY DATA SHEET

Creation Date 22-Jun-2009 **Revision Date** 19-Dec-2025 **Revision Number** 8

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name **2,2,4-Trimethylpentane**

Cat No. : **AC421980000; AC421980025; AC421980040; AC421985000**

CAS No 540-84-1
Synonyms Isooctane

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company
Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

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

2. Hazard(s) identification

Classification
This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Flammable liquids	Category 2
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Central nervous system (CNS).	
Aspiration Toxicity	Category 1

Label Elements

Signal Word
Danger

Hazard Statements
Highly flammable liquid and vapor
May be fatal if swallowed and enters airways
Causes skin irritation
Causes serious eye irritation
May cause drowsiness or dizziness

Precautionary Statements
Prevention
Wash face, hands and any exposed skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
Keep container tightly closed
Ground and bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Keep cool
Take action to prevent static discharges
Use non-sparking tools
Response
Get medical attention/advice if you feel unwell
Inhalation
IF INHALED: Remove person to fresh air and keep comfortable for breathing
Call a POISON CENTER or doctor if you feel unwell
Skin
If skin irritation occurs: Get medical advice/attention
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
Take off contaminated clothing and wash before reuse
Eyes
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention
Ingestion
IF SWALLOWED: Immediately call a POISON CENTER or doctor
Do NOT induce vomiting
Fire
In case of fire: Use CO2, dry chemical, or foam to extinguish
Storage
Store locked up
Store in a well-ventilated place. Keep container tightly closed
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)
Very toxic to aquatic life with long lasting effects

Hazards classified under paragraph (d)(1)(ii) of 1910.1200
No information available

3. Composition/information on Ingredients

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

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

Notes to Physician Treat symptomatically

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.

Unsuitable Extinguishing Media Water may be ineffective, Do not use a solid water stream as it may scatter and spread fire

Flash Point -12 °C / 10.4 °F

Method - No information available

Autoignition Temperature 410 °C / 770 °F

Explosion Limits

Upper 6.0 vol %

Lower 1.1 vol %

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge No information available

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.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO_2).

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.

NFPA

Health	Flammability	Instability	Physical hazards
3	3	0	N/A

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.

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. Incompatible Materials. Strong oxidizing agents. Strong acids. Strong bases.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Isooctane	TWA: 300 ppm			TWA: 300 ppm

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

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.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 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.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State Liquid

Color Colorless

Odor	Petroleum distillates	
Odor Threshold	No information available	
Property	**Values**	**Remarks • Method**
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
Flammability (liquid)	Highly flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	**Lower** 1.1 vol % **Upper** 6 vol %	
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)	

Other Information

Molecular Formula	C8 H18
Molecular Weight	114.23
Explosive Properties	Vapors may form explosive mixtures with air

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

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

Incompatible Materials Strong oxidizing agents, Strong acids, Strong bases

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

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation Irritating to respiratory system. May be harmful if inhaled. INHALATION MAY CAUSE CENTRAL NERVOUS SYSTEM EFFECTS.

Ingestion May be harmful if swallowed. Aspiration hazard. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea. Harmful if swallowed. Potential for aspiration if swallowed.

Eyes Irritating to eyes.

Skin Irritating to skin. May be harmful in contact with skin.

Toxicology data for the components

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

Toxicologically Synergistic Products No information available

(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

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Isooctane	540-84-1	Not listed	Not listed	Not listed	Not listed	Not listed

(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.

Other Adverse Effects The toxicological properties have not been fully investigated.

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

12. Ecological information

Ecotoxicity

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 Algae	Freshwater Fish	Microtox	Water Flea
Isooctane	EC50= 2.94 mg/l, 72h	LC50 = 0.11 mg/l, 96h,	Not listed	EC50= 0.4 mg/l, 48h

		(Rainbow trout)		(Daphnia magna)

Persistence and Degradability Insoluble in water Persistence is unlikely based on information available. Immiscible with water

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its volatility. Is not likely mobile in the environment due its low water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

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

TDG

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

IMDG/IMO

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

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Isooctane	540-84-1	X	ACTIVE	-

Legend:
TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)
X - Listed
'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories
Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL

Isooctane	540-84-1	X	-	208-759-1	X	X	X	X	X	KE-34634

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

U.S. Federal Regulations

SARA 313
Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories
Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
Isooctane	X		-

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA
This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355).

Component	Hazardous Substances RQs	CERCLA Extremely Hazardous Substances RQs	SARA Reportable Quantity (RQ)
Isooctane	1000 lb	-	1000 lb 454 kg

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Isooctane	X	X	X	X	-

U.S. Department of Transportation
Reportable Quantity (RQ): Y
DOT Marine Pollutant Y
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade Serious risk, Grade 3

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	REACH Regulation (EC 1907/2006) article 59 - Candidate List of

			Substances	Substances of Very High Concern (SVHC)
Isooctane	540-84-1	-	Use restricted. See entry 75. (see link for restriction details)	-

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

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Isooctane	540-84-1	Listed	Not applicable	Not applicable	Not applicable

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

Other International Regulations

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	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Isooctane	540-84-1	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By
Product stewardship (Regulatory Affairs)
Acros Organics BVBA
Tel: 800-ACROS-01

Creation Date 22-Jun-2009
Revision Date 19-Dec-2025
Print Date 19-Dec-2025
Revision Summary Updated to the U.S. Department of Labor’s Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

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 SDS