

SAFETY DATA SHEET

Creation Date 26-Sep-2009

Revision Date 25-Mar-2024

Revision Number 2

1. Identification

Product Name 2-Methylhexane, 99%

Cat No. : 96627

CAS No 591-76-4
Synonyms Isoheptane.

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

Details of the supplier of the safety data sheet

Company

Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757

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 by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2
Skin Corrosion/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
May cause drowsiness or dizziness

Causes skin irritation



Precautionary Statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Keep cool

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician 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/shower
Wash contaminated clothing 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/physician
Do NOT induce vomiting

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

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

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Isoheptane	591-76-4	99

4. First-aid measures

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. Get medical attention.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Aspiration into lungs can produce severe lung damage. Get medical attention. Risk of serious damage to the lungs (by aspiration).
Ingestion	Do NOT induce vomiting. Aspiration hazard. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.
Most important symptoms and effects	Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Causes central nervous system depression
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Carbon dioxide (CO ₂). Dry chemical. Water mist may be used to cool closed containers. Chemical foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	-3 °C / 26.6 °F
Method -	No information available
Autoignition Temperature	220 °C / 428 °F
Explosion Limits	
Upper	6.00%
Lower	1.00%
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Flammable. 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 (CO₂).

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
3

Flammability
3

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required. 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 (e.g. sand, silica gel, acid binder, universal binder, sawdust). 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	Ensure adequate ventilation. Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Take precautionary measures against static discharges. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Wash hands before breaks and immediately after handling the product. Keep away from open flames, hot surfaces and sources of ignition. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded.
Storage.	Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Flammables area. Keep container tightly closed in a dry and well-ventilated place.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Isoheptane	TWA: 400 ppm STEL: 500 ppm			TWA: 400 ppm STEL: 500 ppm

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

Engineering Measures	Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment.
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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	No protective equipment is needed under normal use conditions.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	Petroleum distillates
Odor Threshold	No information available
pH	Not applicable
Melting Point/Range	No data available -118 °C / -180.4 °F
Boiling Point/Range	90 °C / 194 °F @ 760 mmHg
Flash Point	-3 °C / 26.6 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	6.00%
Lower	1.00%
Vapor Pressure	66 mmHg @ 25 °C
Vapor Density	3.45 (Air = 1.0)
Specific Gravity	0.670
Solubility	Immiscible
Partition coefficient; n-octanol/water	No data available

Autoignition Temperature	220 °C / 428 °F
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C7 H16
Molecular Weight	100.2

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Strong oxidizing agents
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

Acute Toxicity

Product Information No acute toxicity information is available for this product

Component Information

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	Irritating to eyes, respiratory system and skin
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Isoheptane	591-76-4	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Central nervous system (CNS)

STOT - repeated exposure None known

Aspiration hazard Category 1

Symptoms / effects, both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Causes central nervous system depression

Endocrine Disruptor Information No information available

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

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.

Persistence and Degradability	Insoluble in water Persistence is unlikely based on information available. Immiscible with water
Bioaccumulation/ Accumulation	No information available.
Mobility	Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility.

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.
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14. Transport information

DOT

UN-No	UN1993
Proper Shipping Name	Flammable liquid, n.o.s.
Technical Name	Isoheptane
Hazard Class	3
Packing Group	II

TDG

UN-No	UN1993
Proper Shipping Name	Flammable liquid, n.o.s.
Hazard Class	3
Packing Group	II

IATA

UN-No	UN1993
Proper Shipping Name	Flammable liquid, n.o.s.
Hazard Class	3
Packing Group	II

IMDG/IMO

UN-No	UN1993
Proper Shipping Name	Flammable liquid, n.o.s.
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
Isoheptane	591-76-4	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/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Isoheptane	591-76-4	X	-	209-730-6	X	X	X	-	X	KE-24218

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 Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

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
Isoheptane	X	-	X	-	-

U.S. Department of Transportation

Reportable Quantity (RQ): N
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 No information available

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
Isoheptane	591-76-4			

			Substances	Substances of Very High Concern (SVHC)
Isoheptane	591-76-4	-	Use restricted. See item 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)
Isoheptane	591-76-4	Not applicable	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)
Isoheptane	591-76-4	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By

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Creation Date

26-Sep-2009

Revision Date

25-Mar-2024

Print Date

25-Mar-2024

Revision Summary

New emergency telephone response service provider.

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