

SAFETY DATA SHEET

Revision Date 01-Apr-2024

Revision Number 3

1. Identification

Product Name	Sulfur in Isooctane standard solution, Specpure®, 10 myg/g (0.0010%)
Cat No. :	41315
Synonyms	No information available
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
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
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 %
Isooctane	540-84-1	99.999
Butane, 1,1'-thiobis-	544-40-1	0.001

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	Difficulty in breathing. 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	Carbon dioxide (CO ₂). Powder. Water spray. In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	-12 °C / 10.4 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Do not allow run-off from fire-fighting to enter drains or water courses.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides.

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	-

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. 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 container tightly closed in a dry and well-ventilated place. Keep away from heat, sparks and flame. Incompatible Materials. Acids. Strong bases. Oxidizing agent.

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 Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment.

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.

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	No information available
Melting Point/Range	No data available
Boiling Point/Range	No information available
Flash Point	-12 °C / 10.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available

Vapor Pressure	23 hPa @ 20 °C
Vapor Density	No information available
Specific Gravity	No information available
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available

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	Acids, Strong bases, Oxidizing agent
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Sulfur oxides
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Oral LD50	Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.
Dermal LD50	Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.
Vapor LC50	Based on ATE data, the classification criteria are not met. ATE > 20 mg/l.

Component Information

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
Butane, 1,1'-thiobis-	LD50 = 2220 mg/kg (Rat)	Not listed	Not listed

Toxicologically Synergistic Products	No information available
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Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
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
Isooctane	540-84-1	Not listed	Not listed	Not listed	Not listed	Not listed
Butane, 1,1'-thiobis-	544-40-1	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects	No information available
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Reproductive Effects	No information available.
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Developmental Effects	No information available.
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Teratogenicity	No information available.
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STOT - single exposure	Central nervous system (CNS)
STOT - repeated exposure	None known
Aspiration hazard	No information available
Symptoms / effects, both acute and delayed	Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
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.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Isooctane	EC50= 2.94 mg/l, 72h	LC50 = 0.11 mg/l, 96h, (Rainbow trout)	Not listed	EC50= 0.4 mg/l, 48h (Daphnia magna)
Butane, 1,1'-thiobis-	Not listed	LC50: = 3.58 mg/L, 96h flow-through (Pimephales promelas)	Not listed	Not listed

Persistence and Degradability	Immiscible with water
Bioaccumulation/ Accumulation	No information available.
Mobility	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.
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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	-
Butane, 1,1'-thiobis-	544-40-1	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/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
Isooctane	540-84-1	X	-	208-759-1	X	X	X	X	X	KE-34634
Butane, 1,1'-thiobis-	544-40-1	X	-	208-870-5	X	X	X	X	X	-

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

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 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)	-
Butane, 1,1'-thiobis-	544-40-1	-	-	-

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
Butane, 1,1'-thiobis-	544-40-1	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)
Isooctane	540-84-1	Not applicable	Not applicable	Not applicable	Not applicable
Butane, 1,1'-thiobis-	544-40-1	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By	Health, Safety and Environmental Department Email: chem.techinfo@thermofisher.com www.thermofisher.com
Revision Date	01-Apr-2024
Print Date	01-Apr-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