

**SAFETY DATA SHEET**

Revision Date 01-Apr-2024

Revision Number 3

**1. Identification**

**Product Name** Sulfur in Isooctane standard solution, Specpure®, 20 µg/g (0.0020%)

**Cat No. :** 45353

**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 CO<sub>2</sub>, 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	100.00
Butane, 1,1'-thiobis-	544-40-1	0.00

### 4. 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>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>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>Most important symptoms and effects</b>	Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
<b>Notes to Physician</b>	Treat symptomatically

## 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	-7 °C / 19.4 °F
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	415 °C / 779 °F
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	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

None known.

### 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

<b>Health</b>	<b>Flammability</b>	<b>Instability</b>	<b>Physical hazards</b>
3	3	0	-

## 6. Accidental release measures

<b>Personal Precautions</b>	Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.
<b>Environmental Precautions</b>	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.

## 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:** Particulates filter conforming to EN 143.

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

## 9. Physical and chemical properties

<b>Physical State</b>	Liquid
<b>Appearance</b>	Colorless
<b>Odor</b>	Petroleum distillates
<b>Odor Threshold</b>	No information available
<b>pH</b>	No information available
<b>Melting Point/Range</b>	-107 °C / -160.6 °F
<b>Boiling Point/Range</b>	98 - 99 °C / 208.4 - 210.2 °F
<b>Flash Point</b>	-7 °C / 19.4 °F
<b>Evaporation Rate</b>	No information available
<b>Flammability (solid,gas)</b>	Not applicable
<b>Flammability or explosive limits</b>	
Upper	No data available
Lower	No data available
<b>Vapor Pressure</b>	23 hPa @ 20 °C

Vapor Density	No information available
Specific Gravity	0.692 g/cm <sup>3</sup>
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	415 °C / 779 °F
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	Strong oxidizing agents
Hazardous Decomposition Products	None under normal use conditions
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
--------------------------------------	--------------------------

### 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
-------------------	--------------------------

Reproductive Effects	No information available.
----------------------	---------------------------

Developmental Effects	No information available.
-----------------------	---------------------------

Teratogenicity	No information available.
----------------	---------------------------

STOT - single exposure	Central nervous system (CNS)
------------------------	------------------------------

<b>STOT - repeated exposure</b>	None known
<b>Aspiration hazard</b>	No information available
<b>Symptoms / effects, both acute and delayed</b>	Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
<b>Endocrine Disruptor Information</b>	No information available
<b>Other Adverse Effects</b>	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 Persistence is unlikely based on information available.

**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.

## 14. Transport information

### DOT

<b>UN-No</b>	UN1262
<b>Proper Shipping Name</b>	OCTANES
<b>Hazard Class</b>	3
<b>Packing Group</b>	II

### TDG

<b>UN-No</b>	UN1262
<b>Proper Shipping Name</b>	OCTANES
<b>Hazard Class</b>	3
<b>Packing Group</b>	II

### IATA

<b>UN-No</b>	UN1262
<b>Proper Shipping Name</b>	OCTANES
<b>Hazard Class</b>	3
<b>Packing Group</b>	II

### IMDG/IMO

<b>UN-No</b>	UN1262
<b>Proper Shipping Name</b>	OCTANES
<b>Hazard Class</b>	3
<b>Packing Group</b>	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**