

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

### 1.1. Product identifier

Product Description: 1,1,1,3,3,3-Hexafluoroacetone sesquihydrate  
Cat No. : 269970000; 269970250  
CAS No 13098-39-0  
Molecular Formula C<sub>3</sub> F<sub>6</sub> O . 1.5 H<sub>2</sub> O

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

Recommended Use Laboratory chemicals.  
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 Pharmaceuticaaan 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

Based on available data, the classification criteria are not met

##### Health hazards

Acute oral toxicity	Category 3 (H301)
Acute dermal toxicity	Category 2 (H310)

# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

Acute Inhalation Toxicity - Vapors  
Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation  
Reproductive Toxicity

Category 3 (H331)  
Category 2 (H315)  
Category 1 (H318)  
Category 2 (H361fd)

## **Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



Signal Word

Danger

## **Hazard Statements**

H310 - Fatal in contact with skin  
H361fd - Suspected of damaging fertility. Suspected of damaging the unborn child  
H315 - Causes skin irritation  
H318 - Causes serious eye damage  
H301 + H331 - Toxic if swallowed or if inhaled

## **Precautionary Statements**

P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P310 - Immediately call a POISON CENTER or doctor/physician  
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P362 - Take off contaminated clothing and wash before reuse  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

## **2.3. Other hazards**

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
2-Propanone, 1,1,1,3,3,3-hexafluoro-, sesquihydrate	13098-39-0		>95	Acute Tox. 3 (H301) Acute Tox. 2 (H310) Acute Tox. 3 (H331) Skin Irrit. 2 (H315) Eye Dam. 1 (H318) Repr. 2 (H361fd)

# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>General Advice</b>	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Inhalation</b>	If breathing is difficult, give oxygen. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Remove to fresh air. Immediate medical attention is required.
<b>Self-Protection of the First Aider</b>	Use personal protective equipment as required.

### 4.2. Most important symptoms and effects, both acute and delayed

Causes burns by all exposure routes. . Causes eye burns. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

### 4.3. Indication of any immediate medical attention and special treatment needed

**Notes to Physician** Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### Suitable Extinguishing Media

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam.

#### Extinguishing media which must not be used for safety reasons

No information available.

### 5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes.

#### Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Gaseous hydrogen fluoride (HF).

### 5.3. Advice for firefighters

# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

## SECTION 6: ACCIDENTAL RELEASE MEASURES

### 6.1. Personal precautions, protective equipment and emergency procedures

Use personal protective equipment as required. Ensure adequate ventilation. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### 6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

### 6.3. Methods and material for containment and cleaning up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

### 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. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

### 7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 6.1A  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific

# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

regulatory bodies

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

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

Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

#### 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 compatibility, 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.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

#### 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 EN14387

#### Small scale/Laboratory use

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 141

When RPE is used a face piece Fit Test should be conducted

# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

Environmental exposure controls No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Off-white	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	18 - 21 °C / 64.4 - 69.8 °F	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	No information available	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	1-2	
Viscosity	0.67 mPa.s at 38 °C	
Water Solubility	Soluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
2-Propanone, 1,1,1,3,3,3-hexafluoro-, sesquihydrate	1.46	
Vapor Pressure	202 hPa @ 30°C	
Density / Specific Gravity	1.690	
Bulk Density	Not applicable	Liquid
Vapor Density	No information available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

### 9.2. Other information

Molecular Formula	C3 F6 O . 1.5 H2 O
Molecular Weight	193.05

## SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity	None known, based on information available
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10.2. Chemical stability	Moisture sensitive.
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### 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. Excess heat. Exposure to moist air or water.
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10.5. Incompatible materials	Strong oxidizing agents.
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# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

## 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Gaseous hydrogen fluoride (HF).

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Product Information

##### (a) acute toxicity;

Oral	Category 3
Dermal	Category 2
Inhalation	Category 3

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 1

##### (d) respiratory or skin sensitization;

Respiratory	No data available
Skin	No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

##### (g) reproductive toxicity; Reproductive Effects

Category 2  
Possible risk of impaired fertility. Possible risk of harm to the unborn child.

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

#### Other Adverse Effects

The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information

#### Symptoms / effects, both acute and delayed

Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated. Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation.

### 11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any

# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

#### Ecotoxicity effects

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

### 12.2. Persistence and degradability

#### Persistence

Soluble in water, Persistence is unlikely, based on information available.

### 12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
2-Propanone, 1,1,1,3,3,3-hexafluoro-, sesquihydrate	1.46	No data available

### 12.4. Mobility in soil

The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

### 12.5. Results of PBT and vPvB assessment

No data available for assessment.

### 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.

#### European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

#### Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms.

## SECTION 14: TRANSPORT INFORMATION



# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

## IMDG/IMO

**14.1. UN number** UN2552  
**14.2. UN proper shipping name** HEXAFLUOROACETONE HYDRATE, LIQUID  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** II

## ADR

**14.1. UN number** UN2552  
**14.2. UN proper shipping name** HEXAFLUOROACETONE HYDRATE, LIQUID  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** II

## IATA

**14.1. UN number** UN2552  
**14.2. UN proper shipping name** HEXAFLUOROACETONE HYDRATE, LIQUID  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** II

**14.5. Environmental hazards** No hazards identified

**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/NDL), 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
2-Propanone, 1,1,1,3,3,3-hexafluoro-, sesquihydrate	13098-39-0	-	-	-	X	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDL	AICS	NZIoC	PICCS
2-Propanone, 1,1,1,3,3,3-hexafluoro-, sesquihydrate	13098-39-0	-	-	-	-	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 Not applicable

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)
2-Propanone,	13098-39-0	-	-	-

# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

1,1,1,3,3,3-hexafluoro-, sesquihydrate				
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## 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
2-Propanone, 1,1,1,3,3,3-hexafluoro-, sesquihydrate	13098-39-0	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)?**

See table for values

Component	OECD PFAS	US (EPA) PFAS	EU (ECHA) PFAS	UK (HSE) PFAS	Chemsec PFAS (Sin List)
2-Propanone, 1,1,1,3,3,3-hexafluoro-, sesquihydrate (CAS #: 13098-39-0)	-	-	Listed	Listed	-

### PFAS Legend

Listed = Meets the PFAS definition of the named authority

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 .

Take note of Directive 94/33/EC on the protection of young people at work

Take note of Dir 92/85/EC on the protection of pregnant and breastfeeding women at work

## National Regulations

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

### WGK Classification

Water endangering class = 3 (self classification)

## 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

H331 - Toxic if inhaled

H301 - Toxic if swallowed

H310 - Fatal in contact with skin

H315 - Causes skin irritation

H318 - Causes serious eye damage

H361fd - Suspected of damaging fertility. Suspected of damaging the unborn child

# SAFETY DATA SHEET

1,1,1,3,3,3-Hexafluoroacetone sesquihydrate

Revision Date 29-Sep-2023

## 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

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer 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

### **Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**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)

### **Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Creation Date** 16-Nov-2010  
**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.**

### **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**