

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

# 1,1,1,3,3,3-Hexafluoro-2-propanol



Version number: 2  
Issued: 2024-03-13

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1. Product identifier

**Trade name**

1,1,1,3,3,3-Hexafluoro-2-propanol

**CAS number**

920-66-1

**EC number**

213-059-4

**Synonyms**

Bis(trifluoromethyl)-methanol

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

**Relevant identified uses**

Research and development. Laboratory Chemicals. Manufacture of substances.

**Not suitable for use in**

Not suitable for human consumption or veterinary purposes.

### 1.3. Details of the supplier of the safety data sheet

**Supplier**

Molekula Group

Address

Molekula Ltd, Lingfield Way, Darlington,  
DL1 4XX Darlington  
United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

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## 1.4. Emergency telephone number

### Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

#### Classification

Serious eye damage, hazard category 1

Skin corrosion, hazard category 1C

Reproductive toxicity, hazard category 2

Specific Target Organ Toxicity — Repeated exposure, hazard category 2

Acute toxicity, inhalation, hazard category 4

Acute toxicity, dermal, hazard category 4

Acute toxicity, oral, hazard category 4

#### Hazard statements

H302 + H312 + H332, H314, H318, H361, H373

### 2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

#### Hazard pictograms



#### Signal word

Danger

#### Hazard statements

H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.

H314 Causes severe skin burns and eye damage.

H361 Suspected of damaging fertility or the unborn child.

H373 May cause damage to organs through prolonged or repeated exposure.

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## Precautionary statements

P201 Obtain special instructions before use.  
P202 Do not handle until all safety precautions have been read and understood.  
P261 Avoid breathing dust/fumes/gas/mist/vapours/spray.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P310 Immediately call a POISON CENTER/doctor.  
P312 Call a POISON CENTER/doctor if you feel unwell.  
P314 Get medical advice/attention if you feel unwell.  
P321 Specific treatment (see on this label).  
P363 Wash contaminated clothing before reuse.  
P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.  
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.  
P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P308 + P313 IF exposed or concerned: Get medical advice/attention.  
P405 Store locked up.  
P501 Dispose of contents/container to local regulations.

## 2.3. Other hazards

No data available

## SECTION 3: Composition/information on ingredients

### 3.2. Mixtures

| Chemical name                     | CAS No.<br>EC No.<br>REACH No.<br>Index No. | Concentration | Classification   | H-phrases<br>M factor acute<br>M factor chronic               | Note |
|-----------------------------------|---|---------------|--|---|------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol | 920-66-1<br>213-059-4<br>-<br>-             | 100%          | Acute Tox. 4 -<br>inhalation, Skin<br>Corr. 1C, Eye<br>Dam. 1, Repr. 2,<br>STOT RE 2 | H302 + H312 +<br>H332, H314,<br>H318, H361,<br>H373<br>-<br>- | -    |

## Molecular weight

168.04

## Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

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## SECTION 4: First aid measures

### 4.1. Description of first aid measures

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel.

#### Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary.

#### Skin contact

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. Immediately call a POISON CENTER/doctor.

#### Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

#### Ingestion

IF SWALLOWED: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only if the persons are fully conscious and awake). Administer activated charcoal (20 - 40g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

#### Information for doctors

No data available.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure. Causes burns by all exposure routes.

See section 11 for more detailed information on health effects and symptoms.

#### Inhalation

Single exposure may cause the following adverse effects: Causes severe burns. Difficulty in breathing. Unconsciousness, possibly death.

#### Skin contact

Single exposure may cause the following adverse effects: Causes severe burns. Blistering may occur. May be absorbed in the body and cause dizziness, nausea and vomiting. Unconsciousness, death.

#### Eye contact

Single exposure may cause the following adverse effects: Causes serious eye damage. Unconsciousness, possibly death.

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## Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. May cause severe internal injury. Unconsciousness, possibly death.

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

Treat symptomatically. Immediately call a POISON CENTER/doctor.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

#### Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

#### Unsuitable extinguishing media

No specific fire fighting procedure given.

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

Specific hazards: Corrosive. Combustible.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

Hydrogen fluoride (HF).

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3. Advice for firefighters

#### Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Prevent skin contact by maintaining a safe distance and by wearing suitable protective equipment/ clothing. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

## SECTION 6: Accidental release measures

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

Do not breathe vapour/spray. Avoid contact with skin and eyes. For personal protection, see section 8.

In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

### 6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

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

Collect with absorbent, non-combustible material into suitable containers.

### 6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

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## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### Preventive handling precautions

For precautions see section 2.2. Work under hood Take action to prevent static discharges. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Avoid ingestion and inhalation.

#### General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Wash contaminated skin thoroughly after handling. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use.

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

Store in a dry place. Store in a closed container.

Recommended storage temperature: 2 to 8°C (35.6 to 46.4°F )

### 7.3. Specific end use(s)

No specific usage precautions noted.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No data available

### 8.2. Exposure controls

#### Personal Protective Equipment Symbols



#### Eye / face protection

Wear eye protection.

#### Hand protection

Wear protective gloves. Recommended gloves: Viton rubber (fluor rubber).

Glove Thickness: 0.7mm

Breakthrough time: 8 hours

Do NOT use: Butyl rubber.

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

#### Other skin protection

Wash skin thoroughly after handling.

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## Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

## Environmental exposure controls

Avoid discharge into drains.

## SECTION 9: Physical and chemical properties

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

#### Physical state

Liquid

#### Colour

Colourless.

#### Odour

Aromatic.

#### Melting point / freezing point

-2 °C

#### Boiling point or initial boiling point and boiling range

59 °C

#### Flammability

No data available

#### Lower and upper explosion limit

No data available

#### Flash point

No data available

#### Auto-ignition temperature

> 550 °C

#### Decomposition temperature

59 °C

#### pH

No data available

#### Kinematic viscosity

No data available

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## Solubility

No data available

## Partition coefficient n-octanol/water

1.5

## Vapour pressure

No data available

## Density and/or relative density

1.596

## Relative vapour density

No data available

## Particle characteristics

No data available

## 9.2. Other information

No data available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

There are no known reactivity hazards associated with this product.

### 10.2. Chemical stability

Stable under the prescribed storage conditions.

### 10.3. Possibility of hazardous reactions

No data available

### 10.4. Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
Incompatible materials.

### 10.5. Incompatible materials

Strong oxidising agents. Strong acids. Strong bases Aluminium. Zinc. Alkali metals. Butyl rubber.  
Alcohols Amines. Nitrogen oxides Oxygen. Copper. Powdered metal.

### 10.6. Hazardous decomposition products

See section 5.

## SECTION 11: Toxicological information

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

#### Acute toxicity



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| Product / Substance name<br>CAS / EC no.                  | Dose descriptor | Value / Dose | Exposure route | Test animals |
|---|-----------------|--------------|----------------|--------------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | LD50            | 1500 mg/kg   | Oral           | Rat          |
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | LC50            | 1974ppm      | Inhalation.    | Rat          |
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | LD50            | 1400 mg/kg   | Dermal         | Rabbit       |

## Skin corrosion/irritation

| Product / Substance name<br>CAS / EC no.                  | Result     | Species |
|---|------------|---------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | Corrosive. | Rabbit  |

## Serious eye damage/irritation

| Product / Substance name<br>CAS / EC no.                  | Result                     | Species |
|---|----------------------------|---------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | Causes serious eye damage. | Rabbit  |

## Respiratory or skin sensitisation

| Product / Substance name<br>CAS / EC no.                  | Result    | Species | Method / Guideline     |
|---|-----------|---------|------------------------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | Negative. | Mouse   | Local Lymph Node Assay |

## Germ cell mutagenicity

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| Product / Substance name<br>CAS / EC no.                  | Result    | Metabolic activation /<br>Exposure    | Species                                 | Method / Guideline |
|---|-----------|---------------------------------------|---|--------------------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | Negative. | with and without metabolic activation | Escherichia coli/Salmonella typhimurium | Ames test          |

## Reproductive toxicity

| Product / Substance name<br>CAS / EC no.                  | Result   |
|---|--|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | Suspected of damaging fertility. Suspected of damaging the unborn child. |

## STOT-repeated exposure

| Product / Substance name<br>CAS / EC no.                  | Exposure route | Result   |
|---|----------------|--|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | Oral           | May cause damage to organs through prolonged or repeated exposure. |

## Aspiration hazard

Based on available data, the classification criteria are not met.

## 11.2. Information on other hazards

No data available

## SECTION 12: Ecological information

### 12.1. Toxicity

#### Acute fish toxicity

| Product / Substance name<br>CAS / EC no.                  | Measurement type | Value / Result | Duration of exposure | Species                                  |
|---|------------------|----------------|----------------------|--|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | LC50             | 244.0 mg/l     | 96 hours             | Pimephales promelas<br>(Fat-head Minnow) |

#### Acute algae toxicity

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| Product / Substance name<br>CAS / EC no.                  | Measurement type | Value / Result | Duration of exposure | Species                         |
|---|------------------|----------------|----------------------|---------------------------------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | NOEC             | ≥100 mg/l      | 72 hours             | Pseudokirchneriella subcapitata |
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | ErC50            | >100 mg/l      | 72 hours             | Pseudokirchneriella subcapitata |

**Acute crustacean toxicity**

| Product / Substance name<br>CAS / EC no.                  | Measurement type | Value / Result | Duration of exposure | Species       |
|---|------------------|----------------|----------------------|---------------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | EC50             | >97.3 mg/l     | 48 hours             | Daphnia magna |

**12.2. Persistence and degradability**

**Persistence and degradability**

| Product / Substance name<br>CAS / EC no.                  | Type of test | Duration | Result | Degradation                               |
|---|--------------|----------|--------|---|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | aerobic      | 28 days  | 0-5%   | The product is not readily biodegradable. |

**12.3. Bioaccumulative potential**

**Bioaccumulative potential**

| Product / Substance name<br>CAS / EC no.                  | Duration | Result | Species                       |
|---|----------|--------|-------------------------------|
| 1,1,1,3,3,3-Hexafluoro-2-propanol<br>920-66-1 / 213-059-4 | 42 days  | 1 mg/l | Cyprinus carpio (Common carp) |

**12.4. Mobility in soil**

No data available

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## 12.5. Results of PBT and vPvB assessment

No data available

## 12.6. Endocrine disrupting properties

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

## 12.7. Other adverse effects

No data available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

#### Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

## SECTION 14: Transport information

### 14.1. UN number

3265

### 14.2. UN proper shipping name

#### ADR / RID / ADN proper shipping name

CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (1,1,1,3,3,3-Hexafluoro-2-propanol)

#### IMDG proper shipping name

CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (1,1,1,3,3,3-Hexafluoro-2-propanol)

#### IATA proper shipping name

Corrosive liquid, acidic, organic, n.o.s. (1,1,1,3,3,3-Hexafluoro-2-propanol)

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## 14.3. Transport hazard class(es)

### Label

ADR/RID/ADN



8

IMDG



8

IATA



8

### ADR / RID Class

8

### ADR / RID Classification code

C3

### ADR / RID hazard identification number

88

### IMDG Class

8

### IATA Class

8

### ADN Class

8

### ADN Class Code

CJ

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## 14.4. Packing group

ADR / RID / ADN: I  
IMDG: I  
IATA: I

## 14.5. Environmental hazards

Not applicable

## 14.6. Special precautions for user

### Special precautions for user

Tunnel restriction code: E  
Transport category: 1

### IMDG EmS

F-A, S-B

## 14.7. Maritime transport in bulk according to IMO instruments

Not applicable

## SECTION 15: Regulatory information

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

#### EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.  
This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

#### National regulations

No data available

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

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## SECTION 16: Other information

### Phrase meaning

Eye Dam. 1 - Serious eye damage, hazard category 1

Skin Corr. 1C - Skin corrosion, hazard category 1C

Repr. 2 - Reproductive toxicity, hazard category 2

STOT RE 2 - Specific Target Organ Toxicity — Repeated exposure, hazard category 2

Acute Tox. 4 - inhalation - Acute toxicity, inhalation, hazard category 4

Acute Tox. 4 - dermal - Acute toxicity, dermal, hazard category 4

Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4

H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.

H314 Causes severe skin burns and eye damage.

H318 Causes serious eye damage.

H361 Suspected of damaging fertility or the unborn child.

H373 May cause damage to organs through prolonged or repeated exposure.