

**1,1,1,3,3,3-Hexafluoro-2-propanol ≥99 %, for (peptide) synthesis**

article number: **2473**  
Version: **GHS 1.0 en**

date of compilation: 2016-08-24

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

### 1.1 Product identifier

Identification of the substance	<b>1,1,1,3,3,3-Hexafluoro-2-propanol</b>
Article number	2473
Registration number (REACH)	This information is not available.
EC number	213-059-4
CAS number	920-66-1

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

**Identified uses:** laboratory chemical

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

Carl Roth GmbH + Co KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:** +49 (0) 721 - 56 06 0

**Telefax:** +49 (0) 721 - 56 06 149

**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

**e-mail (competent person)** : [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification according to Regulation (EC) No 1272/2008 (CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

### 2.2 Label elements

#### Labelling according to Regulation (EC) No 1272/2008 (CLP)

not required

**Signal word** not required

### 2.3 Other hazards

There is no additional information.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	1,1,1,3,3,3-Hexafluoro-2-propanol
EC number	213-059-4
CAS number	920-66-1
Molecular formula	C3H2F6O
Molar mass	168 g/mol

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off contaminated clothing.

#### Following inhalation

Provide fresh air. If breathing is irregular or stopped, administer artificial respiration. Call a physician immediately.

#### Following skin contact

Call a physician immediately.

#### Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

#### Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

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

Symptoms and effects are not known to date

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

none

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings  
water spray, foam, dry extinguishing powder, carbon dioxide (CO<sub>2</sub>)

#### Unsuitable extinguishing media

water jet

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

Solvent vapours are heavier than air and may spread along floors. Combustible.

#### Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>), hydrogen fluoride (HF)

### 5.3 Advice for firefighters

Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

## SECTION 6: Accidental release measures

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

#### For non-emergency personnel

Wipe up with absorbent material (e.g. cloth, fleece). Do not breathe vapour/spray.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water.

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

#### Advices on how to contain a spill

Covering of drains.

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

#### Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

No special measures are necessary.

#### Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

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

Keep container tightly closed.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Consideration of other advice

##### • Ventilation requirements

Use local and general ventilation.

##### • Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C.

### 7.3 Specific end use(s)

No information available.

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

#### Occupational exposure limit values (Workplace Exposure Limits)

No data available.

### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)



#### Eye/face protection

Use safety goggles with side protection.

#### Skin protection

##### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374.

##### • type of material

FKM: fluoro-elastomer

##### • material thickness

> 0,7mm.

##### • breakthrough times of the glove material

>480 minutes (permeation: level 6)

##### • other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

#### Respiratory protection

Type: AX (gas filters and combined filters against low-boiling point organic compounds, colour code: Brown).

#### Environmental exposure controls

Keep away from drains, surface and ground water.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

#### Appearance

Physical state	liquid (fluid)
Colour	colourless
Odour	characteristic
Odour threshold	No data available

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### Other physical and chemical parameters

pH (value)	2 - 4 (20 °C) aqueous solution of the substance
Melting point/freezing point	-3 - -2 °C
Initial boiling point and boiling range	59 °C at 1,013 hPa
Flash point	>100 °C
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)

### Explosive limits

• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	not relevant

Vapour pressure	160 hPa at 20 °C 269 hPa at 30 °C
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Density	1.62 g/cm <sup>3</sup> at 20 °C
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Vapour density	This information is not available.
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Bulk density	Not applicable
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Relative density	Information on this property is not available.
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### Solubility(ies)

Water solubility	soluble
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### Partition coefficient

n-octanol/water (log KOW)	1.66
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Auto-ignition temperature	Information on this property is not available.
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Decomposition temperature	no data available
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### Viscosity

• dynamic viscosity	1.65 mPa s at 20 °C
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Explosive properties	Shall not be classified as explosive
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Oxidising properties	none
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## 9.2 Other information

Solvent content	100 %
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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

In case of warming: Vapours can form explosive mixtures with air

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

Violent reaction with: Oxidisers, Alkali metals, Bases, Strong acid, Aluminium, Acid halides, Zinc

### 10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Source
inhalation: vapour	LC50	13.8 mg/l/4h	rat	
oral	LD50	1,500 mg/kg	rat	

#### Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

#### Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

#### Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

#### Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

#### • Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

#### • Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

#### Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

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### Symptoms related to the physical, chemical and toxicological characteristics

- **If swallowed**

If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects)

- **If in eyes**

data are not available

- **If inhaled**

cough, Dyspnoea

- **If on skin**

data are not available

### Other information

None

## SECTION 12: Ecological information

### 12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

#### Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
LC50	244 mg/l	Pimephales promelas		96 h

### 12.2 Process of degradability

Theoretical Oxygen Demand: 0.5713 mg/mg  
Theoretical Carbon Dioxide: 0.7857 mg/mg

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)

1.66

BCF

1.1 - 1.4 (1.1 - 1.4)

### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Other adverse effects

Data are not available.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

Consult the appropriate local waste disposal expert about waste disposal.

#### Sewage disposal-relevant information

Do not empty into drains.

#### Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

### 13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

### 13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

## SECTION 14: Transport information

14.1	UN number	3265
14.2	UN proper shipping name	<b>CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.</b>
	Hazardous ingredients	1,1,1,3,3,3-Hexafluoro-2-propanol
14.3	Transport hazard class(es)	
	Class	8 (corrosive substances)
14.4	Packing group	II (substance presenting medium danger)
14.5	Environmental hazards	none (non-environmentally hazardous acc. to the dangerous goods regulations)
14.6	<b>Special precautions for user</b>	
	Provisions for dangerous goods (ADR) should be complied within the premises.	
14.7	<b>Transport in bulk according to Annex II of MARPOL and the IBC Code</b>	
	The cargo is not intended to be carried in bulk.	
14.8	<b>Information for each of the UN Model Regulations</b>	
	<b>• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)</b>	
	UN number	3265
	Proper shipping name	CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.
	Particulars in the transport document	UN3265, CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S., (1,1,1,3,3,3-Hexafluoro-2-propanol ), 8, II, (E)
	Class	8
	Classification code	C3
	Packing group	II
	Danger label(s)	8



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Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Tunnel restriction code (TRC)	E
Hazard identification No	80
<b>Emergency Action Code</b>	2X

### • International Maritime Dangerous Goods Code (IMDG)

UN number	3265
Proper shipping name	CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.
Particulars in the shipper's declaration	UN3265, CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S., (1,1,1,3,3,3-Hexafluoro-2-propanol), 8, II
Class	8
Packing group	II
Danger label(s)	8



Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-A, S-B
Stowage category	B
Segregation group	1 - Acids

## SECTION 15: Regulatory information

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

#### Relevant provisions of the European Union (EU)

- Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)  
Not listed.

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- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**

Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**

Not listed.

- **Restrictions according to REACH, Annex XVII**

not listed

- **List of substances subject to authorisation (REACH, Annex XIV)**

not listed

- **Limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products (2004/42/EC, Deco-Paint Directive)**

VOC content 100 %

- **Directive on industrial emissions (VOCs, 2010/75/EU)**

VOC content 100 %

- **Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II**

not listed

- **Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)**

not listed

- **Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)**

not listed

### National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- REACH (Europe)

## 15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

## SECTION 16: Other information

### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
BCF	BioConcentration Factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule

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Abbr.	Descriptions of used abbreviations
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IMDG	International Maritime Dangerous Goods Code
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds
vPvB	very Persistent and very Bioaccumulative

### Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)

### List of relevant phrases (code and full text as stated in chapter 2 and 3)

not relevant.

### Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.