

SAFETY DATA SHEET

according to 1907/2006/EC, Article 3

Version no. : 2.1
Prepared on : 30.03.2019
Revised on : 23.09.2025

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

1.1 Product identifiers

Product name 4,4,4-Trifluorobutan-1-ol
Product Number PSR50193
Brand PureSynth research chemicals
CAS No. 461-18-7

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

Identified uses : Laboratory Reagent

1.3 Details of the supplier of the safety data sheet

Company PureSynth Research Chemicals GmbH.
64683 Einhausen Marie-Curie-StraBe. 3, Germany

1.4 Emergency telephone number

Worldwide Helpline No.: 1800-8908-260

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Flammable liquids, (Category 3) H226: Flammable liquid and vapor.

Acute toxicity, (Category 4) H302: Harmful if swallowed.

Eye irritation, (Category 2) H319: Causes serious eye irritation.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal word Warning

Hazard statement(s)

H226 Flammable liquid and vapor.

H302 Harmful if swallowed.

H319 Causes serious eye irritation.

Precautionary statement(s)

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources.
No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P301 + P312 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.

P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

2.3 Other hazards: This substance/mixture contains no components considered to be either persistent, bio accumulative and toxic (PBT), or very persistent and very bio accumulative (vPvB) at levels of 0.1% or higher.

Ecological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition / information on ingredients

3.1 Substances

Common names & Synonyms	Mol. formula	CAS number
4,4,4-Trifluoro-n-butanol	C ₄ H ₇ F ₃ O	461-18-7
Component	Classification	Concentration
4,4,4-trifluor-1-butanol	Flam. Liq. 3; Acute Tox. 4; Eye Irrit. 2; H226, H302, H319	<= 100 %

SECTION 4: First aid measures

Description of first aid measures

General advice	Show this material safety data sheet to the doctor in attendance.
If inhaled	After inhalation: fresh air.
In case of skin contact	Take off immediately all contaminated clothing. Rinse skin with water/shower.
In case of eye contact	Rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.
If swallowed	After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
Most important symptoms and effects, both acute and delayed	The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
Indication of any immediate medical attention and special treatment needed	No data available

SECTION 5: Fire fighting measures

Extinguishing media	
Suitable extinguishing media	Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	For this substance/mixture no limitations of extinguishing agents are given.
Special hazards arising from the substance or mixture	Carbon oxides Hydrogen fluoride Combustible. Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air at elevated temperatures. Development of hazardous combustion gases or vapours possible in the event of fire.
Advice for fire-fighters	In the event of fire, wear self-contained breathing apparatus.

Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

**Environmental precautions
Methods and materials for containment and cleaning up**

Do not let product enter drains. Risk of explosion. Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material. Dispose of properly. Clean up affected area.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on protection against fire and explosion: Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures: Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Heat sensitive.

Storage class (TRGS 510): 3: Flammable liquids.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls / Personal protection

Control parameters

Ingredients with workplace control parameters

Exposure controls

Personal protective equipment:

Eye / face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses. required

Skin protection

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Appearance	Form: Liquid
	Colour: No data available
Odour	No data available
pH - Value	No data available
Density	1.2117 g/cm ³
Boiling Point	123 - 127 °C
Melting Point	No data available
Solubility in water	No data available
Flash point	50.6 °C
Vapour pressure	No data available
Auto-ignition temperature	No data available
Vapour density	No data available
Flammability (solid, gas)	No data available
Evaporation rate	No data available
Partition coefficient: n- octanol / water	log Pow: 0.707
Viscosity	No data available
Explosive properties	No data available
Upper / lower flammability or explosive limits	No data available
Oxidizing properties	none

Other safety information: No data available

SECTION 10: Stability and reactivity

Reactivity	Vapor/air-mixtures are explosive at intense warming.
Chemical stability	The product is chemically stable under standard ambient conditions (room temperature)
Possibility of hazardous reactions	No data available
Condition to avoid	Heating.
Incompatible materials	Strong acids and oxidizing agents.
Hazardous decomposition products	In the event of fire: see section 5.

SECTION 11: Toxicological information

Acute toxicity	Oral: No data available Inhalation: No data available Dermal: No data available
Skin corrosion/irritation	No data available .
Serious eye damage/eye irritation	No data available
Respiratory or skin sensitization	No data available
Germ cell mutagenicity	No data available
Carcinogenicity	No data available
Reproductive toxicity	No data available
Specific target organ toxicity - single exposure	No data available

Specific target organ toxicity - repeated exposure No data available
Aspiration hazard No data available

Additional Information

Endocrine disrupting properties

Assessment The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 12: Ecological information

Toxicity No data available
Persistence and degradability No data available
Bio accumulative potential No data available
Mobility in soil No data available
Results of PBT and vPvB assessment This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.
Endocrine disrupting properties The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
Other adverse effects Avoid release to the environment.

SECTION 13: Disposal considerations

Waste treatment methods products No data available

SECTION 14: Transport information

	UN no.	UN proper shipping name	Hazard Class(es)	Packaging group	Marine Pollutant
ADR / RID	1993	FLAMMABLE LIQUID, N.O.S. (4,4,4-trifluor-1-butanol)	3	III	No
IMDG	1993	FLAMMABLE LIQUID, N.O.S. (4,4,4-trifluor-1-butanol)	3	III	No
IATA	1993	Flammable liquid, n.o.s. (4,4,4-trifluor-1-butanol)	3	III	No

SECTION 15: Regulatory information

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

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

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council P5c FLAMMABLE LIQUIDS on the control of major-accident hazards involving dangerous substances.

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable. Take note of Dir 94/33/EC on the protection of young people at work.

Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

The information in this SDS is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. The user must be determined suitability of this information for his application.