

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 21.11.2010

Version 3.4

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

1.1 Product identifier

Catalogue No.	841244
Product name	4-Hydroxybenzotrifluoride for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merck-chemicals.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Specific target organ toxicity - single exposure, Category 3, H335

Skin irritation, Category 2, H315

Eye irritation, Category 2, H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

Xi; R36/37/38

For the full text of the R-phrases mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Warning

Hazard statements

H315 Causes skin irritation.

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H319 Causes serious eye irritation.
H335 May cause respiratory irritation.

Precautionary statements

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word
Warning

CAS-No. 402-45-9

Labelling (67/548/EEC or 1999/45/EC)

Symbol(s) Xi Irritant

R-phrases 36/37/38 Irritating to eyes, respiratory system and skin.

EC-No. 206-945-7

Reduced labelling (≤125 ml)

Symbol(s) Xi Irritant

2.3 Other hazards

None known.

3. Composition/information on ingredients

Formula	C ₇ H ₅ F ₃ O (Hill)
CAS-No.	402-45-9
EC-No.	206-945-7
Molar mass	162,11 g/mol

4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, Cough, Shortness of breath

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4.3 Indication of immediate medical attention and special treatment needed

No information available.

5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible material, Vapours are heavier than air and may spread along floors., Forms explosive mixtures with air on intense heating., Development of hazardous combustion gases or vapours possible in the event of fire., Fire may cause evolution of:

Hydrogen fluoride

5.3 Advice for firefighters

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Avoid inhalation of dusts. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7.2 and 10.5).

Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

Indications about waste treatment see section 13.

7. Handling and storage

7.1 Precautions for safe handling

Observe label precautions.

7.2 Conditions for safe storage, including any incompatibilities

May decompose, especially when stored over long periods. Tightly closed. Dry.

Store below +15°C.

7.3 Specific end uses

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

8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet(>,<) supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment:

protective clothing

Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 1 (acc. to DIN 3181) for solid particles of inert substances

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.

Environmental exposure controls

Do not empty into drains.

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9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	powder, finecrystalline
Colour	white
Odour	No information available.
Odour Threshold	No information available.
pH	No information available.
Melting point	46 - 48 °C
Boiling point/boiling range	73 - 75 °C at 11 hPa
Flash point	83 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Relative density	No information available.
Water solubility	No information available.
Partition coefficient: n-octanol/water	log Pow: 2,82 Method: (experimental) (Lit.) No remarkable bioaccumulation potential is expected (log Pow 1-3).
Autoignition temperature	No information available.
Decomposition temperature	130 °C
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Oxidizing properties	No information available.

9.2 Other data

none

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10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

The following applies in general to flammable organic substances and preparations: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents, Acid anhydrides, Bases, polymerisation, Hydrogen fluoride, alkalines

10.4 Conditions to avoid

Strong heating (explosive decomposition).

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See chapter 5.

11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute inhalation toxicity

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Skin irritation

Causes skin irritation.

Eye irritation

Causes serious eye irritation.

Specific target organ toxicity - single exposure

May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

11.2 Further information

Further information

Quantitative data on the toxicity of this product are not available.

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,82

Method: (experimental)

(Lit.) No remarkable bioaccumulation potential is expected (log Pow 1-3).

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information

We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

Do not allow to run into surface waters, wastewater, or soil.

13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

14. Transport information

Not classified as dangerous in the meaning of transport regulations.

15. Regulatory information

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

EU regulations

Major Accident Hazard 96/82/EC

Legislation Directive 96/82/EC does not apply

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work.

National legislation

Storage class VCI 10 - 13 Other liquids and solids

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

16. Other information

Full text of H-Statements referred to under sections 2 and 3.

H315 Causes skin irritation.

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Product name	4-Hydroxybenzotrifluoride for synthesis

H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

Full text of R-phrases referred to under sections 2 and 3

R36/37/38	Irritating to eyes, respiratory system and skin.
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Training advice

Provide adequate information, instruction and training for operators.

Regional representation:	This information is given on the authorised Safety Data Sheet for your country.
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Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.