

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 23.07.2018

Version 2.5

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

### 1.1 Product identifier

Catalogue No.	814964
Product name	1-Bromo-4-(trifluoromethoxy)benzene for synthesis
REACH Registration Number	1-2120747298-43-XXXX
CAS-No.	407-14-7

### 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 ( <a href="http://www.merckgroup.com">www.merckgroup.com</a> ).

### 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: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

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

### 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Skin irritation, Category 2, H315

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

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## 2.2 Label elements

### Labelling (REGULATION (EC) No 1272/2008)

#### *Hazard pictograms*



#### *Signal word*

Warning

#### *Hazard statements*

H315 Causes skin irritation.

#### *Precautionary statements*

##### Prevention

P260 Do not breathe vapours.

P262 Do not get in eyes, on skin, or on clothing.

##### Response

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

### Reduced labelling ( $\leq 125$ ml)

#### *Hazard pictograms*



#### *Signal word*

Warning

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## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	C <sub>7</sub> H <sub>4</sub> BrF <sub>3</sub> O (Hill)
EC-No.	206-979-2
Molar mass	241,01 g/mol

### Hazardous components (REGULATION (EC) No 1272/2008)

*Chemical name (Concentration)*

CAS-No.	Registration number	Classification
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1-bromo-4-(trifluoromethoxy)benzene (<= 100 % )

407-14-7	1-2120747298-43-XXXX	Skin irritation, Category 2, H315
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For the full text of the H-Statements mentioned in this Section, see Section 16.

### 3.2 Mixture

Not applicable

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## SECTION 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.

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

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

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

#### *Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), 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.

Vapours 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.

Fire may cause evolution of:

Hydrogen fluoride, hydrogen bromide

### 5.3 Advice for firefighters

#### *Special protective equipment for firefighters*

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.

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## SECTION 6. Accidental release measures

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

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. 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

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The Safety Data Sheets for catalogue items are available at [www.merckgroup.com](http://www.merckgroup.com)

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

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

## 6.4 Reference to other sections

Indications about waste treatment see section 13.

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## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

#### *Advice on safe handling*

Observe label precautions.

#### *Hygiene measures*

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

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

#### *Storage conditions*

Tightly closed.

Recommended storage temperature see product label.

### 7.3 Specific end use(s)

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

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## SECTION 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.

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## 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.

### *Eye/face protection*

Safety glasses

### *Hand protection*

full contact:

Glove material:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 30 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 890 Vitoject® (full contact), KCL 730 Camatril® -Velours (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](http://www.kcl.de)).

### *Other protective equipment*

protective clothing

### *Respiratory protection*

required when vapours/aerosols are generated.

Recommended Filter type: filter 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

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properly documented.

## Environmental exposure controls

Do not empty into drains.

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## SECTION 9. Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Form	liquid
Colour	light brown
Odour	unpleasant
Odour Threshold	No information available.
pH	No information available.
Melting point	No information available.
Boiling point/boiling range	91 - 92 °C at 100 hPa
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.

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Vapour pressure	20 hPa at 55 °C
Relative vapour density	No information available.
Density	1,62 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.
Water solubility	11,7 mg/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 3,93 (calculated) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

none

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## SECTION 10. Stability and reactivity

### 10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

### 10.2 Chemical stability



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

## 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

## 10.4 Conditions to avoid

Heating.

## 10.5 Incompatible materials

no information available

## 10.6 Hazardous decomposition products

in the event of fire: See section 5.

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LD50 Rat: > 2.500 mg/kg

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

(External MSDS)

#### *Acute inhalation toxicity*

This information is not available.

#### *Acute dermal toxicity*

This information is not available.

#### *Skin irritation*

Rabbit

Result: Irritations

(External MSDS)

Causes skin irritation.

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## *Eye irritation*

Rabbit

Result: No eye irritation

(External MSDS)

## *Sensitisation*

This information is not available.

## *Germ cell mutagenicity*

### *Genotoxicity in vitro*

Ames test

Result: negative

(External MSDS)

## *Carcinogenicity*

This information is not available.

## *Reproductive toxicity*

This information is not available.

## *Teratogenicity*

This information is not available.

## *Specific target organ toxicity - single exposure*

This information is not available.

## *Specific target organ toxicity - repeated exposure*

This information is not available.

## *Aspiration hazard*

This information is not available.

## **11.2 Further information**

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## **SECTION 12. Ecological information**

### **12.1 Toxicity**

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## *Toxicity to fish*

LC0 Danio rerio (zebra fish): > 11,7 mg/l; 96 h

(above the solubility limit in the test medium) (External MSDS)

## *Toxicity to bacteria*

EC50 activated sludge: 6.440 mg/l

OECD Test Guideline 209

## **12.2 Persistence and degradability**

### *Biodegradability*

1 %

OECD Test Guideline 301D

Not readily biodegradable.

## **12.3 Bioaccumulative potential**

### *Partition coefficient: n-octanol/water*

log Pow: 3,93

(calculated)

Bioaccumulation is not expected.

## **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*

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

### *Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14. Transport information

### Land transport (ADR/RID)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)

14.1 UN number UN 3334

14.2 Proper shipping name AVIATION REGULATED LIQUID, N.O.S. (1-BROMO-4-(TRIFLUOROMETHOXY)-BENZENE)

14.3 Class 9

14.4 Packing group III

14.5 Environmentally hazardous --

14.6 Special precautions for user no

### Sea transport (IMDG)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

### 14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

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## SECTION 15. Regulatory information

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

#### *EU regulations*

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Major Accident Hazard SEVESO III

Legislation Not applicable

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

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of  $\geq 0.1$  % (w/w).

*National legislation*

Storage class 10 - 13

## 15.2 Chemical safety assessment

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

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## SECTION 16. Other information

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

H315 Causes skin irritation.

### Training advice

Provide adequate information, instruction and training for operators.

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## Labelling

*Hazard pictograms*



*Signal word*

Warning

*Hazard statements*

H315 Causes skin irritation.

*Precautionary statements*

Response

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

P313 Get medical advice/ attention.

## 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](http://www.wikipedia.org).

## Regional representation

This information is given on the authorised Safety Data Sheet for your country.

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*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.*