

Safety Data Sheet

according to UK REACH Regulation

3-Chloro-1-(trifluormethyl)benzene-13C6

Revision date: 19.03.2026

Product code: OP335

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

1.1. Product identifier

3-Chloro-1-(trifluormethyl)benzene-13C6

Further trade names

1-Chloro-3-(trifluoromethyl)benzene-13C6

CAS No: na

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

Use of the substance/mixture

Reference standard for analysis.

1.3. Details of the supplier of the safety data sheet

Company name: WITEGA Laboratorien Berlin-Adlershof GmbH
Street: James-Franck-Strasse 4
Place: D-12489 Berlin
Telephone: +493063922001 Telefax: +493063922007
E-mail: witega@witega.de
Internet: www.witega.de

1.4. Emergency telephone number:

+493063922001

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

GB CLP Regulation

Hazard Statements:
Flammable liquid and vapour.
Causes skin irritation.
Causes serious eye irritation.

2.2. Label elements

GB CLP Regulation

Signal word: Danger

Pictograms:



Hazard statements

H226 Flammable liquid and vapour.
H315 Causes skin irritation.
H319 Causes serious eye irritation.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P262 Do not get in eyes, on skin, or on clothing.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves/protective clothing and eye protection/face protection.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

2.3. Other hazards

No data available

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SECTION 3: Composition/information on ingredients

3.2. Mixtures

Sum formula: C13C6H4ClF3
Molecular weight: 186.51 g/mol g/mol

Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
na	3-Chloro-1-(trifluormethyl)benzene-13C6			100 %
	Flam. Liq. 3, Skin Irrit. 2, Eye Irrit. 2; H226 H315 H319			

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
na		3-Chloro-1-(trifluormethyl)benzene-13C6	100 %
	oral: LD50 = 5000 mg/kg		

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

After inhalation

Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

After contact with skin

Remove contaminated, saturated clothing immediately. Subsequently wash off with: Water and soap

After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

After ingestion

Rinse mouth immediately and drink plenty of water. Get immediate medical advice/attention.
Do NOT induce vomiting. Never give anything by mouth to an unconscious person or a person with cramps.

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

No data available

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

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Water spray jet. Foam. Dry extinguishing powder. Carbon dioxide (CO2).

5.2. Special hazards arising from the substance or mixture

In case of fire may be liberated: Pyrolysis products, toxic. In case of fire and/or explosion do not breathe fumes.

5.3. Advice for firefighters

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In case of fire: Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Use personal protection equipment. Do not breathe gas/fumes/vapour/spray.

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

Other information

Take up dust-free and set down dust-free.

6.4. Reference to other sections

Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation should be used if possible.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.

Advice on general occupational hygiene

Use personal protection equipment.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed in a cool, well-ventilated place. Avoid: UV-radiation/sunlight

Further information on storage conditions

storage temperature: 2-8°C

7.3. Specific end use(s)

none

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.2. Exposure controls

Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation should be used if possible. If local exhaust ventilation is not possible or not sufficient, the entire working area should be ventilated by technical means.

Individual protection measures, such as personal protective equipment

Eye/face protection

Eye glasses with side protection

Hand protection

Wear suitable gloves. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances.

Skin protection

lab coat

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	liquid:		
Colour:	colourless		
Boiling point or initial boiling point and boiling range:		138-140 °C	Test method
Flammability:		No data available	
Lower explosion limits:		No data available	
Upper explosion limits:		No data available	
Flash point:		No data available	
Auto-ignition temperature:		No data available	
Decomposition temperature:		No data available	
pH-Value:		No data available	
Water solubility:		No data available	
Solubility in other solvents			
No data available			
Partition coefficient n-octanol/water:		No data available	OECD (TG) 117
Vapour pressure:		No data available	
Vapour pressure:			DIN 51640
Density (at 25 °C):		1.331 g/cm ³	
Relative vapour density:		No data available	

9.2. Other information

Information with regard to physical hazard classes

Self-ignition temperature	
Solid:	No data available
Gas:	No data available

Other safety characteristics

Evaporation rate:	No data available
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SECTION 10: Stability and reactivity

10.1. Reactivity

Reacts with : Oxidising agent, Alkali (lye), Etchant and acids

10.2. Chemical stability

The product is chemically stable under recommended conditions of storage, use and temperature.

10.3. Possibility of hazardous reactions

No known hazardous reactions.

10.4. Conditions to avoid

Do not expose to temperatures exceeding 50 °C/122 °F.

10.5. Incompatible materials

Oxidising agent, Alkali (lye), Etchant and acids

10.6. Hazardous decomposition products

In case of fire may be liberated: Pyrolysis products, toxic.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in GB CLP Regulation

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Acute toxicity

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

ATEmix calculated

ATE (oral) > 2000 mg/kg; ATE (dermal) > 2000 mg/kg; ATE (inhalation vapour) > 20 mg/l; ATE (inhalation dust/mist) > 5 mg/l

CAS No	Chemical name					
	Exposure route	Dose	Species	Source	Method	
na	3-Chloro-1-(trifluormethyl)benzene-13C6					
	oral	LD50 mg/kg	5000	Rat		

Irritation and corrosivity

Skin corrosion/irritation: Causes skin irritation.

Serious eye damage/eye irritation: Causes serious eye irritation.

Sensitising effects

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

Carcinogenic/mutagenic/toxic effects for reproduction

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

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

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

STOT-single exposure

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

STOT-repeated exposure

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

Aspiration hazard

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

Specific effects in experiment on an animal

No data available

SECTION 12: Ecological information

12.1. Toxicity

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

No data available

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
na	3-Chloro-1-(trifluormethyl)benzene-13C6					
	Acute fish toxicity	LC50 mg/l	70,7	96 h	Danio rerio (zebrafish)	

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No indication of bioaccumulation potential.

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

The substances in the mixture do not meet the PBT/vPvB criteria according to UK REACH.

This substance does not meet the PBT/vPvB criteria of REACH, Annex XIII.

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12.6. Endocrine disrupting properties

This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Dispose of waste according to applicable legislation.

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

Contaminated packaging

This material and its container must be disposed of as hazardous waste.

SECTION 14: Transport information

Land transport (ADR/RID)

<u>14.1. UN number or ID number:</u>	UN 1993
<u>14.2. UN proper shipping name:</u>	FLAMMABLE LIQUID, N.O.S.
<u>14.3. Transport hazard class(es):</u>	3
<u>14.4. Packing group:</u>	II
Hazard label:	3



Classification code:	F1
Special Provisions:	274 601 640C
Limited quantity:	1 L
Excepted quantity:	E2
Transport category:	2
Hazard No:	33
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

<u>14.1. UN number or ID number:</u>	UN 1993
<u>14.2. UN proper shipping name:</u>	FLAMMABLE LIQUID, N.O.S.
<u>14.3. Transport hazard class(es):</u>	3
<u>14.4. Packing group:</u>	II
Hazard label:	3



Classification code:	F1
Special Provisions:	274 601 640C
Limited quantity:	1 L
Excepted quantity:	E2

Marine transport (IMDG)

<u>14.1. UN number or ID number:</u>	UN 1993
<u>14.2. UN proper shipping name:</u>	FLAMMABLE LIQUID, N.O.S.
<u>14.3. Transport hazard class(es):</u>	3
<u>14.4. Packing group:</u>	II
Hazard label:	3

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Special Provisions: 274
 Limited quantity: 1 L
 Excepted quantity: E2
 EmS: F-E, S-E

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 1993
14.2. UN proper shipping name: FLAMMABLE LIQUID, N.O.S.
14.3. Transport hazard class(es): 3
14.4. Packing group: II
 Hazard label: 3



Special Provisions: A3
 Limited quantity Passenger: 1 L
 Passenger LQ: Y341
 Excepted quantity: E2
 IATA-packing instructions - Passenger: 353
 IATA-max. quantity - Passenger: 5 L
 IATA-packing instructions - Cargo: 364
 IATA-max. quantity - Cargo: 60 L

14.6. Special precautions for user

No transport as bulk according to IBC Code.

14.7. Maritime transport in bulk according to IMO instruments

No transport as bulk according to IBC Code.

SECTION 15: Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):
 Entry 40

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information

Abbreviations and acronyms

Flam. Liq: Flammable liquids
 Skin Irrit: Skin irritation
 Eye Irrit: Eye irritation

Relevant H and EUH statements (number and full text)

H226 Flammable liquid and vapour.

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H315 Causes skin irritation.
H319 Causes serious eye irritation.

Further Information

This information is based on our present state of knowledge. However, it should not constitute a guarantee for any specific product properties and shall not establish a legally valid relationship. The substances are only for R&D. Do not use as a drug, in household or other applications.

(The data for the relevant ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)