

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

# 1,3,5-Benzenetricarboxylic acid chloride



Version number: 2  
Issued: 2024-02-07  
Replaces SDS: 2021-11-01

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

### 1.1. Product identifier

**Trade name**

1,3,5-Benzenetricarboxylic acid chloride

**CAS number**

4422-95-1

**EC number**

224-594-8

**Synonyms**

Benzene-1,3,5-tricarbonyl trichloride

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

**Relevant identified uses**

Research and development. Laboratory Chemicals. Manufacture of substances.

**Not suitable for use in**

Not suitable for human consumption or veterinary purposes.

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

**Supplier**

Molekula Group

**Address**

Molekula Ltd, Lingfield Way, Darlington,  
DL1 4XX Darlington  
United Kingdom

**Telephone**

+44 (0) 3302 000 333

**Email**

info@molekula.com

**Web site**

www.molekula.com

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## 1.4. Emergency telephone number

### Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

#### Classification

Skin corrosion, hazard category 1B

Skin sensitisation, hazard category 1

Corrosive to metals, hazard category 1

#### Hazard statements

H290, H314, H317

#### Supplemental hazard statements

EUH014, EUH029

### 2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

#### Hazard pictograms



#### Signal word

Danger

#### Hazard statements

H290 May be corrosive to metals.

H314 Causes severe skin burns and eye damage.

H317 May cause an allergic skin reaction.

#### Supplemental hazard statements

EUH014 Reacts violently with water.

EUH029 Contact with water liberates toxic gas.

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## Precautionary statements

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

P234 Keep only in original packaging.

P260 Do not breathe dust/fumes/gas/mist/vapours/spray.

P264 Wash skin thoroughly after handling.

P272 Contaminated work clothing should not be allowed out of the workplace.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.

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

P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

P304 + P340 IF INHALED: Remove person to fresh air and keep 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.

P310 Immediately call a POISON CENTER/doctor.

P321 Specific treatment (see on this label).

P333 +P313 If skin irritation or rash occurs: Get medical advice/attention.

P363 Wash contaminated clothing before reuse.

P390 Absorb spillage to prevent material damage.

P405 Store locked up.

P406 Store in corrosive resistant container with a resistant inner liner.

P501 Dispose of contents/container to local regulations.

## 2.3. Other hazards

No data available

## SECTION 3: Composition/information on ingredients

### 3.2. Mixtures

| Chemical name                            | CAS No.<br>EC No.<br>REACH No.<br>Index No. | Concentration | Classification                                  | H-phrase<br>M factor acute<br>M factor chronic   | Note |
|--|---|---------------|---|--|------|
| 1,3,5-Benzenetricarboxylic acid chloride | 4422-95-1<br>224-594-8<br>-<br>-            | 100%          | Met. Corr. 1, Skin<br>Corr. 1B, Skin<br>Sens. 1 | H290, H314,<br>H317, EUH014,<br>EUH029<br>-<br>- | -    |

### Molecular weight

265.48

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## **Substance additional information**

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

## **SECTION 4: First aid measures**

### **4.1. Description of first aid measures**

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel.

#### **Inhalation**

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary. Maintain an open airway. Loosen any tight clothing, such as a collar, tie or belt. Rinse nose, mouth and throat with water. Never give anything by mouth to an unconscious person. IF exposed or concerned: Get medical advice/attention.

#### **Skin contact**

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. Immediately call a POISON CENTER/doctor.

#### **Eye contact**

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

#### **Ingestion**

IF SWALLOWED: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only if the persons are fully conscious and awake). Administer activated charcoal (20 - 40g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

#### **Information for doctors**

No data available.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure. Causes burns by all exposure routes.

See section 11 for more detailed information on health effects and symptoms.

#### **Inhalation**

Single exposure may cause the following adverse effects: Causes severe burns. Difficulty in breathing. Unconsciousness, possibly death.

#### **Skin contact**

Single exposure may cause the following adverse effects: Causes severe burns. Blistering may occur. May be absorbed in the body and cause dizziness, nausea and vomiting. Unconsciousness, death.

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## **Eye contact**

Single exposure may cause the following adverse effects: Causes serious eye damage. Unconsciousness, possibly death.

## **Ingestion**

Single exposure may cause the following adverse effects: Severe abdominal pain. May cause severe internal injury. Unconsciousness, possibly death.

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

Treat symptomatically. Immediately call a POISON CENTER/doctor.

## **SECTION 5: Firefighting measures**

### **5.1. Extinguishing media**

#### **Suitable extinguishing media**

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

#### **Unsuitable extinguishing media**

Do not use water jet as an extinguisher, as this will spread the fire.

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

Specific hazards: Corrosive.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

Hydrochloric acid (HCl).

### **5.3. Advice for firefighters**

#### **Special protective equipment for fire-fighters**

Evacuate area. Avoid breathing gas, fume, vapours or spray. Prevent skin contact by maintaining a safe distance and by wearing suitable protective equipment/ clothing. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

## **SECTION 6: Accidental release measures**

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

Do not breathe vapour/spray. Avoid contact with skin and eyes. For personal protection, see section 8.

### **6.2. Environmental precautions**

Avoid discharge into drains, water courses or onto the ground. The product may affect the acidity (pH-factor) in water with risk of harmful effects to aquatic organisms.

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

Collect with absorbent, non-combustible material into suitable containers.

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## 6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### Preventive handling precautions

For precautions see section 2.2. Work under hood. Take action to prevent static discharges. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Avoid ingestion and inhalation.

#### General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Wash contaminated skin thoroughly after handling. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use.

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

Store in a dry place. Store in a closed container.

Store at ambient temperature.

Handle and store contents under inert gas.

### 7.3. Specific end use(s)

No specific usage precautions noted.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No data available

### 8.2. Exposure controls

#### Personal Protective Equipment Symbols



#### Eye / face protection

Wear eye protection.

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## **Hand protection**

Wear protective gloves. Recommended gloves: Viton rubber (fluor rubber).

Glove Thickness: 0.7mm

Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

## **Other skin protection**

Wash skin thoroughly after handling.

## **Respiratory protection**

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

## **Environmental exposure controls**

Avoid discharge into drains.

## **SECTION 9: Physical and chemical properties**

### **9.1. Information on basic physical and chemical properties**

#### **Physical state**

Solid

#### **Colour**

Yellow.

#### **Odour**

No data available

#### **Melting point / freezing point**

32 - 38 °C

#### **Boiling point or initial boiling point and boiling range**

180 °C

#### **Flammability**

No data available

#### **Lower and upper explosion limit**

No data available

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## Flash point

110 °C

## Auto-ignition temperature

No data available

## Decomposition temperature

No data available

## pH

No data available

## Kinematic viscosity

No data available

## Solubility

Soluble in the following materials: Chloroform. Toluene

## Partition coefficient n-octanol/water

No data available

## Vapour pressure

No data available

## Density and/or relative density

1.487 g/cm<sup>3</sup>

## Relative vapour density

No data available

## Particle characteristics

No data available

## 9.2. Other information

No data available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

May be corrosive to metals.

### 10.2. Chemical stability

Stable under the prescribed storage conditions.



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## 10.3. Possibility of hazardous reactions

Violent reactions possible with:

Water

Alcohols

Alkalines

Strong oxidising agents.

## 10.4. Conditions to avoid

strong heating Protect from moisture.

## 10.5. Incompatible materials

Strong oxidising agents.

## 10.6. Hazardous decomposition products

See section 5.

## SECTION 11: Toxicological information

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Acute toxicity

| Product / Substance name<br>CAS / EC no.                          | Dose descriptor | Value / Dose | Exposure route |
|---|-----------------|--------------|----------------|
| 1,3,5-Benzenetricarboxylic acid chloride<br>4422-95-1 / 224-594-8 | LD50            | >2000 mg/kg  | Oral           |

#### Skin corrosion/irritation

| Product / Substance name<br>CAS / EC no.                          | Result             |
|---|--------------------|
| 1,3,5-Benzenetricarboxylic acid chloride<br>4422-95-1 / 224-594-8 | Causes skin burns. |

#### Serious eye damage/irritation

| Product / Substance name<br>CAS / EC no.                          | Result                     |
|---|----------------------------|
| 1,3,5-Benzenetricarboxylic acid chloride<br>4422-95-1 / 224-594-8 | Causes serious eye damage. |

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## Respiratory or skin sensitisation

| Product / Substance name<br>CAS / EC no.                          | Result                               |
|---|--------------------------------------|
| 1,3,5-Benzenetricarboxylic acid chloride<br>4422-95-1 / 224-594-8 | May cause an allergic skin reaction. |

## Aspiration hazard

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

### 11.2. Information on other hazards

No data available

## SECTION 12: Ecological information

### 12.1. Toxicity

No data available

### 12.2. Persistence and degradability

No data available

### 12.3. Bioaccumulative potential

No data available

### 12.4. Mobility in soil

No data available

### 12.5. Results of PBT and vPvB assessment

No data available

### 12.6. Endocrine disrupting properties

This product does not contain any known or suspected endocrine disruptors.

### 12.7. Other adverse effects

No data available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

#### Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

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## SECTION 14: Transport information

### 14.1. UN number

3261

### 14.2. UN proper shipping name

#### ADR / RID / ADN proper shipping name

CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (1,3,5-Benzenetricarboxylic acid chloride)

#### IMDG proper shipping name

CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (1,3,5-Benzenetricarboxylic acid chloride)

#### IATA proper shipping name

Corrosive solid, acidic, organic, n.o.s. (1,3,5-Benzenetricarboxylic acid chloride)

### 14.3. Transport hazard class(es)

#### Label

ADR/RID/ADN



8

IMDG



8

IATA



8

#### ADR / RID Class

8

#### ADR / RID Classification code

C4

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## ADR / RID hazard identification number

80

## IMDG Class

8

## IATA Class

8

## ADN Class

8

## ADN Class Code

C4

### 14.4. Packing group

ADR / RID / ADN: II

IMDG: II

IATA: II

### 14.5. Environmental hazards

Not applicable

### 14.6. Special precautions for user

#### Special precautions for user

Tunnel restriction code: E

Transport category: 2

#### IMDG EmS

F-A, S-B

### 14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC08

## SECTION 15: Regulatory information

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

#### EU regulations

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

This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

#### National regulations

No data available

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

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## SECTION 16: Other information

### Phrase meaning

Skin Corr. 1B - Skin corrosion, hazard category 1B  
Skin Sens. 1 - Skin sensitisation, hazard category 1  
Met. Corr. 1 - Corrosive to metals, hazard category 1  
H290 May be corrosive to metals.  
H314 Causes severe skin burns and eye damage.  
H317 May cause an allergic skin reaction.  
EUH014 Reacts violently with water.  
EUH029 Contact with water liberates toxic gas.