

## Chemical Safety Data Sheet MSDS / SDS

**1,3,5-Tri(4-carboxyphenyl)benzene**

Revision Date:2025-07-26 Revision Number:1

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

Product name : 1,3,5-Tri(4-carboxyphenyl)benzene  
CBnumber : CB41454981  
CAS : 50446-44-1  
Synonyms : H3BTB, 1,3,5-tris(4-carboxyphenyl)benzene

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P501 Dispose of contents/container to.....  
P337+P313 IF eye irritation persists: Get medical advice/attention.  
P332+P313 IF SKIN irritation occurs: Get medical advice/attention.  
P321 Specific treatment (see ... on this label).  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.  
Continuerinsing.  
P273 Avoid release to the environment.  
P264 Wash skin thoroughly after handling.  
P264 Wash hands thoroughly after handling.  
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

**Hazard statements**

H410 Very toxic to aquatic life with long lasting effects

H400 Very toxic to aquatic life

H319 Causes serious eye irritation

H315 Causes skin irritation

H228 Flammable solid

---

## SECTION 3: Composition/information on ingredients

### Substance

|              |                                             |
|--------------|---------------------------------------------|
| Product name | : 1,3,5-Tri(4-carboxyphenyl)benzene         |
| Synonyms     | : H3BTB, 1,3,5-tris(4-carboxyphenyl)benzene |
| CAS          | : 50446-44-1                                |
| MF           | : C27H18O6                                  |
| MW           | : 438.43                                    |

---

## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### Special hazards arising from the substance or mixture

Carbon oxides, Sulfur oxides

Mixture with combustible ingredients.

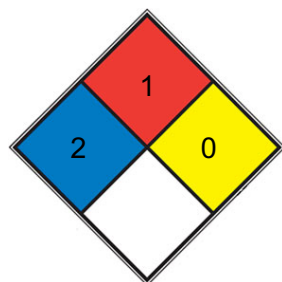
### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

Use water spray to cool unopened containers.

### NFPA 704



**HEALTH** 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

**FIRE** 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

**REACT** 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

**SPEC.**  
**HAZ.**

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

### Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

### Methods and materials for containment and cleaning up

Sweep up and shovel. Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal. Contain spillage, pick up with an electrically protected vacuum cleaner or by wet-brushing and transfer to a container for disposal according to local regulations (see section 13).

### Reference to other sections

For disposal see section 13.

---

## SECTION 7: Handling and storage

### Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

### 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 parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### Body Protection

Impervious clothing, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

---

## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

|                                              |                                                                    |
|----------------------------------------------|--------------------------------------------------------------------|
| Appearance                                   | solid                                                              |
| Odour                                        | No data available                                                  |
| Odour Threshold                              | No data available                                                  |
| pH                                           | No data available                                                  |
| Melting point/freezing point                 | Melting point/range: 322 - 327 °C                                  |
| Initial boiling point and boiling range      | 711.0±60.0 °C(Predicted)                                           |
| Flash point                                  | No data available                                                  |
| Evaporation rate                             | No data available                                                  |
| Flammability (solid, gas)                    | The substance or mixture is a flammable solid with the category 1. |
| Upper/lower flammability or explosive limits | No data available                                                  |
| Vapour pressure                              | No data available                                                  |
| Vapour density                               | No data available                                                  |
| Relative density                             | No data available                                                  |
| Water solubility                             | Soluble in tetrahydrofuran.                                        |
| Partition coefficient: n-octanol/water       | No data available                                                  |
| Autoignition temperature                     | No data available                                                  |
| Decomposition temperature                    | No data available                                                  |
| Viscosity                                    | No data available                                                  |
| Explosive properties                         | No data available                                                  |
| Oxidizing properties                         | No data available                                                  |

### Other safety information

No data available

---

## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

No data available

### Conditions to avoid

Heat, flames and sparks.

### **Incompatible materials**

Oxidizing agents, Strong oxidizing agents, Metals, Amines, Strong acids, Acid chlorides, Alcohols, Peroxides, permanganates, for example potassium permanganate, Strong reducing agents, Soluble carbonates and phosphates, Phosphorus halides, Hydroxides

### **Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulfur oxides

Other decomposition products - No data available In the event of fire: see section 5

---

## **SECTION 11: Toxicological information**

### **Information on toxicological effects**

#### **Acute toxicity**

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**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

#### **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**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

## **SECTION 12: Ecological information**

### **Toxicity**

No data available

### **Persistence and degradability**

No data available

### **Bioaccumulative 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.

### **Other adverse effects**

Very toxic to aquatic life with long lasting effects.

---

## **SECTION 13: Disposal considerations**

### **Waste treatment methods**

#### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

#### **Contaminated packaging**

Dispose of as unused product.

---

## **SECTION 14: Transport information**

### **UN number**

ADR/RID: 3175 IMDG: 3175 IATA: 3175

### **UN proper shipping name**

ADR/RID: SOLIDS CONTAINING FLAMMABLE LIQUID, N.O.S. (acetic acid) IMDG: SOLIDS CONTAINING FLAMMABLE LIQUID, N.O.S. (acetic acid)

IATA: Solids containing flammable liquid, n.o.s. (acetic acid)

### **Transport hazard class(es)**

ADR/RID: 4.1 IMDG: 4.1 IATA: 4.1

### **Packaging group**

ADR/RID: II IMDG: II IATA: II

## Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

## Special precautions for user

No data available

---

# SECTION 15: Regulatory information

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

### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

### Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

EC Inventory:Not Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

---

# SECTION 16: Other information

## Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

## References

【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

【5】ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

**Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.