

SAFETY DATA SHEET

Version 5.3
Revision Date 05/24/2016
Print Date 11/07/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 1,3,5-Tris(4-carboxyphenyl)benzene

Product Number : 686859

Brand : Aldrich

CAS-No. : 50446-44-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable solids (Category 1), H228

Skin corrosion (Category 1A), H314

Serious eye damage (Category 1), H318

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (Category 1), H410

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

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)

H228

Flammable solid.

H314

Causes severe skin burns and eye damage.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210

Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P240

Ground/bond container and receiving equipment.

P241

Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P260

Do not breathe dust or mist.

P264

Wash skin thoroughly after handling.

P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
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.
P310	Immediately call a POISON CENTER/doctor.
P321	Specific treatment (see supplemental first aid instructions on this label).
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P391	Collect spillage.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.2 Mixtures

Synonyms : 4,4',4'',-Benzene-1,3,5-triyl-tris(benzoic acid)
BTB
4,4',4'',-Benzene-1,3,5-triyl-tris(benzoic acid), H3BTB

Formula : C₂₇H₁₈O₆
Molecular weight : 438.43 g/mol

Hazardous components

Component	Classification	Concentration
1,3,5-tris(4-Carboxyphenyl)benzene		
CAS-No. 50446-44-1	Aquatic Acute 1; Aquatic Chronic 1; H410	>= 90 - <= 100 %
Acetic acid		
CAS-No. 64-19-7 EC-No. 200-580-7 Index-No. 607-002-00-6	Flam. Liq. 3; Skin Corr. 1A; Eye Dam. 1; H226, H314, H318	>= 20 - < 30 %
Dimethyl sulfoxide		
CAS-No. 67-68-5 EC-No. 200-664-3	Flam. Liq. 4; H227	>= 20 - < 30 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

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

In case of skin contact

Take off contaminated clothing and shoes immediately. 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. Continue rinsing eyes during transport to hospital.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES**5.1 Extinguishing media****Suitable extinguishing media**

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

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, 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.

6.2 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.

6.3 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).

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

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.

7.2 Conditions for safe storage, including any incompatibilities

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

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Acetic acid	64-19-7	TWA	10.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Pulmonary function Upper Respiratory Tract irritation Eye irritation		
		STEL	15.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Pulmonary function Upper Respiratory Tract irritation Eye irritation		
		ST	15.000000 ppm 37.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Can be found in concentrations of 5-8% in vinegar		
		TWA	10.000000 ppm 25.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Can be found in concentrations of 5-8% in vinegar		
		TWA	10.000000 ppm 25.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	10 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Pulmonary function Upper Respiratory Tract irritation Eye irritation		
		STEL	15 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Pulmonary function Upper Respiratory Tract irritation Eye irritation		
		TWA	10 ppm 25 mg/m3	USA. NIOSH Recommended Exposure Limits
		Can be found in concentrations of 5-8% in vinegar		
		ST	15 ppm 37 mg/m3	USA. NIOSH Recommended Exposure Limits
		Can be found in concentrations of 5-8% in vinegar		
		TWA	10 ppm 25 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		

		PEL	10 ppm 25 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	15 ppm 37 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		C	40 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
Dimethyl sulfoxide	67-68-5	TWA	250.000000 ppm	USA. Workplace Environmental Exposure Levels (WEEL)

Hazardous components without workplace control parameters

8.2 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

Face shield and safety glasses 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.

Body Protection

Complete suit protecting against chemicals, 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|--|--|
| a) Appearance | Form: solid |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: 322 - 327 °C (612 - 621 °F) |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | No data available |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | The substance or mixture is a flammable solid with the category 1. |

j)	Upper/lower flammability or explosive limits	No data available
k)	Vapour pressure	No data available
l)	Vapour density	No data available
m)	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials

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

10.6 Hazardous decomposition products

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

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

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

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

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.

Kidney - Irregularities - Based on Human Evidence

Eyes - Eye disease - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence (Acetic acid)

Eyes - Eye disease - Based on Human Evidence (Dimethyl sulfoxide)

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

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

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 3175 Class: 4.1 Packing group: II
Proper shipping name: Solids containing flammable liquid, n.o.s. (Acetic acid)
Reportable Quantity (RQ): 25000 lbs

Poison Inhalation Hazard: No

IMDG

UN number: 3175 Class: 4.1 Packing group: II EMS-No: F-A, S-I
Proper shipping name: SOLIDS CONTAINING FLAMMABLE LIQUID, N.O.S. (Acetic acid)

IATA

UN number: 3175 Class: 4.1 Packing group: II
Proper shipping name: Solids containing flammable liquid, n.o.s. (Acetic acid)

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Acetic acid	64-19-7	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
1,3,5-tris(4-Carboxyphenyl)benzene	50446-44-1	
Acetic acid	64-19-7	1993-04-24
Dimethyl sulfoxide	67-68-5	2007-03-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
1,3,5-tris(4-Carboxyphenyl)benzene	50446-44-1	
Acetic acid	64-19-7	1993-04-24
Dimethyl sulfoxide	67-68-5	2007-03-01

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

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

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Eye Dam.	Serious eye damage
Flam. Liq.	Flammable liquids
H226	Flammable liquid and vapour.
H227	Combustible liquid.
H228	Flammable solid.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.
Skin Corr.	Skin corrosion

HMIS Rating

Health hazard:	3
Chronic Health Hazard:	*
Flammability:	3
Physical Hazard	3

NFPA Rating

Health hazard:	3
Fire Hazard:	3
Reactivity Hazard:	3

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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