
SECTION 1: Identification

1.1 GHS Product identifier

Product name 2,4,6-trinitrobenzoic acid

1.2 Other means of identification

Product number -

Other names 2,4,6-trinitro-benzoic acid; Trinitrobenzoic acid,dry; 2,4,6-Trinitro-benzoesaeure

1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research uses.

Uses advised against no data available

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

no data available

2.2 GHS label elements, including precautionary statements

Pictogram(s) no data available

Signal word no data available

Hazard statement(s) no data available

Precautionary statement(s)

Prevention no data available

Response no data available

Storage no data available

Disposal no data available

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
2,4,6-trinitrobenzoic acid	2,4,6-trinitrobenzoic acid	129-66-8	204-958-2	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

4.2 Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 112 [Explosives* - Division 1.1, 1.2, 1.3 or 1.5]: Fire may produce irritating, corrosive and/or toxic gases. (ERG, 2016)

Excerpt from ERG Guide 113 [Flammable Solids - Toxic (Wet/Desensitized Explosive)]: Some are toxic and may be fatal if inhaled, swallowed or absorbed through skin. Contact may cause burns to skin and eyes. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

Excerpt from ERG Guide 113 [Flammable Solids - Toxic (Wet/Desensitized Explosive)]: Some are toxic and may be fatal if inhaled, swallowed or absorbed through skin. Contact may cause burns to skin and eyes. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or

place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Organic acids and related compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

If material on fire or involved in fire: Dangerously explosive. Do not fight fires in a cargo of explosives. Evacuate area and let burn. Trinitrobenzoic acid, dry

5.2 Specific hazards arising from the chemical

Excerpt from ERG Guide 112 [Explosives* - Division 1.1, 1.2, 1.3 or 1.5]: MAY EXPLODE AND THROW FRAGMENTS 1600 METERS (1 MILE) OR MORE IF FIRE REACHES CARGO. For information on "Compatibility Group" letters, refer to Glossary section. (ERG, 2016)

Excerpt from ERG Guide 113 [Flammable Solids - Toxic (Wet/Desensitized Explosive)]: Flammable/combustible material. May be ignited by heat, sparks or flames. DRIED OUT material may explode if exposed to heat, flame, friction or shock; treat as an explosive, refer to ERG Guide 112. Keep material wet with water or treat as an explosive, refer to ERG Guide 112. Runoff to sewer may create fire or explosion hazard. (ERG, 2016)

Excerpt from ERG Guide 113 [Flammable Solids - Toxic (Wet/Desensitized Explosive)]: Flammable/combustible material. May be ignited by heat, sparks or flames. DRIED OUT material may explode if exposed to heat, flame, friction or shock; treat as an explosive, refer to ERG Guide 112. Keep material wet with water or treat as an explosive, refer to ERG Guide 112. Runoff to sewer may create fire or explosion hazard. (ERG, 2016)

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

6.2 Environmental precautions

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

6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Trinitrobenzoic acid is a yellow crystalline solid high explosive. Easily ignited and burns vigorously when dry. Insoluble in water. Will burn when wet, although may be difficult to ignite. Produces toxic oxides of nitrogen during combustion. May explode under exposure to heat or fire. Primary hazard is blast of an instantaneous explosion, not flying projectiles or fragments.
Colour	Orthorhombic or rhombohedral crystals from water
Odour	no data available
Melting point/freezing point	228.7Å°C
Boiling point or initial boiling point and boiling range	435.8Å°C at 760mmHg
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	193.6Å°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Soluble in acetone, methanol; slightly soluble in benzene; at 25 deg C: 26.6% in alcohol, 14.7% in ether
Partition coefficient n-octanol/water	log Kow = 0.23 (est)
Vapour pressure	2.3E-08mmHg at 25Å°C
Density and/or relative density	1.87g/cm3
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Highly flammable. Insoluble in water.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

Dry, the material is easily ignited and will burn vigorously. The wet material can burn though it may require some effort to ignite. Aromatic nitro compounds, such as TRINITROBENZOIC ACID, range from slight to strong oxidizing agents. If mixed with reducing agents, including hydrides, sulfides and nitrides, they may begin a vigorous reaction that culminates in a detonation. The aromatic nitro compounds may explode in the presence of a base such as sodium hydroxide or potassium hydroxide even in the presence of water or organic solvents. The explosive tendencies of aromatic nitro compounds are increased by the presence of multiple nitro groups. All heavy metal salts of this compound are explosive on heating or impact.

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Reacts with heavy metals to form heat- or impact-sensitive explosive salts.

10.6 Hazardous decomposition products

Sublimes with decomposition forming CO2 and trinitrobenzene.

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information**12.1 Toxicity**

- Toxicity to fish: no data available
- Toxicity to daphnia and other aquatic invertebrates: no data available
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

12.2 Persistence and degradability

AEROBIC: After 180 minutes, very little oxygen consumption by phenol adapted biological cultures occurred with 2,4,6-trinitrobenzoic acid(1). The amounts of oxygen consumed after the 180 minute test time are 53 uL (endogenous), 61 uL (cells plus 100 mg/L 2,4,6-trinitrobenzoic acid), and 342 uL (cells plus phenol, after 90 minutes) which results in a ratio of only 1.2 endogenous to 2,4,6-trinitrobenzoic acid oxygen consumption(1). The trinitro derivatives of benzoic acid were more readily reduced in the presence of enzyme preparations from *Veillonella alcalescens* than the toluene or phenol derivatives and are degraded more slowly than the mononitro and dinitro derivatives of benzoic acid, toluene, or phenol(2). Three moles of hydrogen are required to reduce each nitro group to the amino group(2). These data suggest that biodegradation is not expected to be an important fate process in the environment(SRC).

12.3 Bioaccumulative potential

An estimated BCF of 3.2 was calculated in fish for 2,4,6-trinitrobenzoic acid(SRC), using an estimated log Kow of 0.23(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 2,4,6-trinitrobenzoic acid can be estimated to be 200(SRC). According to a classification scheme(2), this estimated Koc value suggests that 2,4,6-trinitrobenzoic acid is expected to have moderate mobility in soil. However, the pKa of 2,4,6-trinitrobenzoic acid is 0.65(3), indicating that this compound will almost entirely exist in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4).

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations**13.1 Disposal methods****Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN0215 (For reference only, please check.) IMDG: UN0215 (For reference only, please check.) IATA: UN0215 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: TRINITROBENZOIC ACID, dry or wetted with less than 30% water, by massâ€ (For reference only, please check.) IMDG: TRINITROBENZOIC ACID, dry or wetted with less than 30% water, by massâ€ (For reference only, please check.) IATA: TRINITROBENZOIC ACID, dry or wetted with less than 30% water, by massâ€ (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 1.1D (For reference only, please check.) IMDG: 1.1D (For reference only, please check.) IATA: 1.1D (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: (For reference only, please check.) IMDG: (For reference only, please check.) IATA: (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: No IMDG: No IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
2,4,6-trinitrobenzoic acid	2,4,6-trinitrobenzoic acid	129-66-8	204-958-2
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Not Listed.
China Catalog of Hazardous chemicals 2015			Listed.
New Zealand Inventory of Chemicals (NZIoC)			Not Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Not Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Not Listed.
Korea Existing Chemicals List (KECL)			Not Listed.

SECTION 16: Other information

Information on revision

Creation Date July 15, 2019
Revision Date July 15, 2019

Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:

<http://www.phmsa.dot.gov/hazmat/library/erg>

- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>