

Safety data sheet

according to 1907/2006/EC, Article 31

Printing date 09.04.2021

Version: 3

Revision: 08.04.2021

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

- **1.1 Product identifier**
- **Trade name: Purified terephthalic acid (PTA)**
- **Synonyms:** 1,4-Benzenedicarboxylic acid; para-Phthalic acid; TPA; terephthalic acid; PTA.
- **CAS Number:** 100-21-0
- **EINECS Number:** 202-830-0
- **Registration number** 01-211985970-27-0043
- **1.2 Relevant identified uses of the substance or mixture and uses advised against**
Polyester production, polymer production, manufacturing of organic derivatives, plasticizers, coatings and composite materials, hot-melt adhesives.
- **Application of the substance / the mixture**
Coating compound/ Surface coating/ paint
Intermediate
Monomer
Polymer production
Laboratory chemicals

SECTION 2: Hazards identification

- **2.1 Classification of the substance or mixture**
- **Classification according to Regulation (EC) No 1272/2008**
The substance is not classified, according to the CLP regulation.
- **2.2 Label elements**
- **Labelling according to Regulation (EC) No 1272/2008** Not applicable
- **Hazard pictograms** Not applicable
- **Signal word** Not applicable
- **Hazard statements** Not applicable
- **2.3 Other hazards**
- **Results of PBT and vPvB assessment**
- **PBT:** The substance does not meet the PBT criteria (not PBT) according to (EC) 1907/2006, Annex XIII.
- **vPvB:** The substance does not meet the vPvB criteria (not vPvB) according to (EC) 1907/2006, Annex XIII.

SECTION 3: Composition/information on ingredients

- **3.1 Substances**
- **CAS No.**
100-21-0
- **CAS Description:** 1,3-Benzenedicarboxylic acid
- **Identification number(s)**
- **EC number:** 202-830-0

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- **Impurities and stabilising additives:**
Mono-constituent substance of organic origin.
Impurity content is less than 0.1% by weight and it does not impact the CLP classification of the substance.

SECTION 4: First aid measures

- **4.1 Description of first aid measures**
- **General information:** No special measures required.
- **After inhalation:**
Supply fresh air; consult doctor in case of complaints.
Get medical attention if symptoms appear.
- **After skin contact:**
Immediately wash with water and soap and rinse thoroughly.
Get medical attention if symptoms occur.
- **After eye contact:**
Immediately flush eyes with copious amounts of water for at least 15 minutes.
Get medical attention if irritation occurs.
- **After swallowing:**
Do not induce vomiting; call for medical help immediately.
Do not give anything by mouth to an unconscious person.
If large quantities of this material are swallowed, call a physician immediately
- **4.2 Most important symptoms and effects, both acute and delayed** No further relevant information available.
- **4.3 Indication of any immediate medical attention and special treatment needed**
No further relevant information available.
Treatment should be symptomatic and directed to relieving any effects.

SECTION 5: Firefighting measures

- **5.1 Extinguishing media**
- **Suitable extinguishing agents:**
CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **For safety reasons unsuitable extinguishing agents:** Water with full jet.
- **5.2 Special hazards arising from the substance or mixture**
Carbon dioxide (CO₂)
Fine dust clouds may form explosive mixtures with air.
Handling of this product may generate static electricity, which can present an ignition hazard in some cases.
- **5.3 Advice for firefighters**
- **Protective equipment:**
Wear fully protective suit.
Mouth respiratory protective device.
Fire-fighters should wear self-contained positive pressure breathing apparatus (SCBA) and full turnout gear.
Dynamic risk assessment is to be used throughout mitigation of the incident.

SECTION 6: Accidental release measures

- **6.1 Personal precautions, protective equipment and emergency procedures**
No action shall be taken involving any personal risk or without suitable training.
Evacuate surrounding areas.
Keep unnecessary and unprotected personnel from entering.
Avoid breathing dust.
Do not touch or walk through spilled material.
Provide adequate ventilation.
Wear appropriate respirator when ventilation is inadequate.

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Use appropriate personal protective equipment.

· **6.2 Environmental precautions:**

Do not allow to enter sewers/ surface or ground water.

Eliminate all ignition sources if safe to do so.

Avoid creating dusty conditions and prevent wind dispersal.

Water spray or water fog can be used to remove dust particles from the air.

Do not use water jet.

Wetting the spilled material with water spray or water fog will reduce the amount of airborne dust that is created when the material is cleaned up.

Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

· **6.3 Methods and material for containment and cleaning up:**

Move containers from spill area.

Approach the release from upwind and place in a designated labelled waste container.

Prevent entry into sewers, water courses, basements or confined areas.

Vacuum or sweep up material and place in a designated, labelled waste container.

Dispose of via a licensed waste disposal contractor.

· **6.4 Reference to other sections**

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

SECTION 7: Handling and storage

· **7.1 Precautions for safe handling**

Keep away from heat and direct sunlight.

Prevent formation of dust.

Store in cool, dry place in tightly closed receptacles.

Ensure good ventilation/exhaustion at the workplace.

Wash thoroughly after handling.

· **Information about fire - and explosion protection:**

Protect against electrostatic charges.

To avoid fire or explosion, dissipate static electricity during transfer by earthing and bonding containers and equipment before transferring material.

The need for additional measures for explosion protection should be evaluated.

· **7.2 Conditions for safe storage, including any incompatibilities**

· **Storage:**

· **Requirements to be met by storerooms and receptacles:** Avoid any source of ignition.

· **Information about storage in common storage facility:** Store away from strong oxidizers.

· **Further information about storage conditions:**

Keep container tightly sealed.

Store receptacle in a well ventilated area.

Store in cool, dry conditions in well sealed receptacles.

· **7.3 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

· **8.1 Control parameters**

· **Ingredients with limit values that require monitoring at the workplace:**

CAS: 100-21-0 terephthalic acid

VL (Belgium)	Long-term value: 10 mg/m ³
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AGW (Germany)	Long-term value: 5E mg/m ³ 2(I);Y, DFG
LEP (Spain)	Short-term value: 10 mg/m ³ Long-term value: 5 mg/m ³
TWA (Italy)	Long-term value: 10 mg/m ³
VLE (Portugal)	Long-term value: 10 mg/m ³

· **DNELs****CAS: 100-21-0 terephthalic acid**

Oral	DNEL systemic effects, long-term	3.3 mg/kg bw/day (population)
Dermal	DNEL systemic effects, long-term	33 mg/kg bw/day (population) 67 mg/kg bw/ day (worker)
Inhalative	DNEL systemic effects, long-term	5.8 mg/m ³ (population) 23 mg/m ³ (worker)

· **PNECs****CAS: 100-21-0 terephthalic acid**

PNEC STP	50 mg/l (general)
PNEC freshw sed	0.52 mg/kg sed dw (general)
PNEC freshwater	0.38 mg/l (general)
PNEC saltw sed	0.052 mg/kg sed dw (general)
PNEC saltwater	0.038 mg/l (general)
PNEC soil	0.71 mg/kg soil dw (general)
PNEC intermittent release (freshwater)	1.9 mg/l (general)

· **Additional information:** The lists valid during the making were used as basis.· **8.2 Exposure controls**· **Appropriate engineering controls** Mechanical exhaust required· **Individual protection measures, such as personal protective equipment**· **General protective and hygienic measures:**

The usual precautionary measures are to be adhered to when handling chemicals.

Do not eat, drink, smoke or sniff while working.

Wash hands before breaks and at the end of work.

· **Respiratory protection:**

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use self-contained respiratory protective device.

Filter P2

· **Hand protection**

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation.

· **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

· **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

· **Eye/face protection**

Tightly sealed goggles

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· **Body protection:** Skin and Body: None required; however, use of protective clothing is good industrial practice.

SECTION 9: Physical and chemical properties

· 9.1 Information on basic physical and chemical properties

· General Information

· Colour:	White
· Smell:	Acidic
· Olfactory threshold:	Not determined
· Melting point/freezing point:	402-404 °C (peer-reviewed source)
· Boiling point or initial boiling point and boiling range	sublimes 402-404 °C
· Flammability	Not applicable
· Lower and upper explosion limit	
· Lower:	Not determined
· Upper:	Not determined
· Flash point:	Not applicable
· Auto-ignition temperature:	Not determined
· Decomposition temperature:	Not determined
· pH (0.02 g/l) at 25 °C	3.88
· Viscosity:	
· Kinematic viscosity	Not applicable.
· Dynamic:	Not applicable.
· Solubility	peer reviewed source: 0.013% (w/w) acetic acid 0.10% (w/w) methanol 6.7% (w/w) dimethylformamide 19% (w/w) DMSO
· water at 25 °C:	0.017 g/l
· Partition coefficient n-octanol/water (log value) at 25 °C	2 log POW (QSAR estimation)
· Vapour pressure at 25 °C:	0.002 Pa (QSAR estimation)
· Density and/or relative density	
· Density at 20 °C:	1.58 g/cm ³ (peer-reviewed source)
· Vapour density	Not determined

· 9.2 Other information

· Appearance:	
· Form:	Powder
· Important information on protection of health and environment, and on safety.	
· Explosive properties:	Based on its structure, the product does not present an explosion hazard. The product is not explosive.
· Softening point/range	
· Oxidising properties	According to the structure, this substance has no oxidizing properties.
· Evaporation rate	Not applicable

· Information with regard to physical hazard classes

· Explosives	Not determined
· Flammable gases	Void
· Aerosols	Void
· Oxidising gases	Void
· Gases under pressure	Void
· Flammable liquids	Void

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· Flammable solids	Void
· Self-reactive substances and mixtures	Void
· Pyrophoric liquids	Void
· Pyrophoric solids	Void
· Self-heating substances and mixtures	Void
· Substances and mixtures, which emit flammable gases in contact with water	Void
· Oxidising liquids	Void
· Oxidising solids	Void
· Organic peroxides	Void
· Corrosive to metals	Void
· Desensitised explosives	Void
· Dissociation constant	pk1: 3.62 (25°C) pk2: 4.60 (25°C)

SECTION 10: Stability and reactivity

- **10.1 Reactivity** Stable when applying the recommended regulations for storage and handling.
- **10.2 Chemical stability**
The product is stable under ordinary conditions.
Under normal conditions of storage and use, hazardous polymerization will not occur.
- **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
- **10.3 Possibility of hazardous reactions** No dangerous reactions known.
- **10.4 Conditions to avoid**
Keep away from heat, sparks and open flames.
Static electricity discharge.
Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. No information provided on hazardous wastes.
- **10.5 Incompatible materials:** Strong oxidizing agents
- **10.6 Hazardous decomposition products:** Carbon oxides

SECTION 11: Toxicological information

- **11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008**
- **Acute toxicity** Based on available data, the classification criteria are not met.
- **General information:**

LD/LC50 values relevant for classification:

CAS: 100-21-0 terephthalic acid

Oral	LD50	15,380 mg/kg (rat) (Similar to OECD Guideline 401)
Dermal	LD50	2,000 mg/kg (rabbit) (Similar to OECD Guideline 402)
Inhalative	LC50/4 h	1 mg/L (rat) (Similar to OECD Guideline 403)

- **Skin corrosion/irritation**
Based on available data, the classification criteria are not met.
In vivo studies show that the substance is a mild skin and eye irritant but is not corrosive, and is not classified according to current criteria.
- **Serious eye damage/irritation**
Based on available data, the classification criteria are not met.
The available studies indicate that terephthalic acid is not classified as a skin or eye irritant, or as corrosive, according to CLP Regulation.

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- **Respiratory or skin sensitisation**

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

No evidence of skin sensitisation was noted in a Buehler study with the read-across compound isophthalic acid (IPA). The OECD QSAR Toolbox does not report any structural alerts for protein binding activity (relevant for skin sensitisation) for terephthalic acid.

- **Carcinogenicity**

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

LOAEL: 1000 mg/kg bw/d (equivalent or similar to OECD Guideline 453)

Target organs for carcinogenicity: urogenital: urinary bladder

Humans are generally considered to be less sensitive than rats to urolithiasis for anatomical reasons; it is extremely unlikely that humans could be exposed to the levels of TPA of the magnitude used in the rat toxicity studies, or for similarly long periods.

- **Germ cell mutagenicity**

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

Terephthalic acid is not classified for genotoxicity under CLP, based on the negative results in studies in vivo.

- **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.

Oral NOAEL 125 mg/kg bw/day systemic (rat) (subchronic, 90 day exposure test)

Inhalative NOAEC 10 mg/m³ local (rat) (subacute, OECD Guideline 412, 28/14-Day test)

10 mg/m³ systemic (rat) (subacute, OECD Guideline 412, 28/14-Day test)

- **Aspiration hazard** Based on available data, the classification criteria are not met.

- **Toxicokinetics, metabolism and distribution**

The results of several toxicokinetics studies indicate that terephthalic acid is rapidly absorbed following oral or intratracheal administration and is rapidly excreted in the urine. There is no indication of bioaccumulation. Hoshi and Kuretani (1967); Wolkowski-Tyl et al (1982); Moffitt et al (1975).

- **Reproductive toxicity**

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

CAS: 100-21-0 terephthalic acid

Oral	NOAEL	318 mg/kg bw/day (rat) (Read-across study DEHT/DOTP, Development Tox)
		2010.9 mg/kg bw/day (rat) (subchronic, OECD Guideline 414)
Inhalative	NOAEL	10 mg/m ³ systemic (rat) (subacute, OECD Guideline 412, 28/14-Day test)

- **11.2 Information on other hazards**

- **Endocrine disrupting properties** Substance is not listed.

SECTION 12: Ecological information

- **12.1 Toxicity**

- **Aquatic toxicity:**

The long-term NOECs for freshwater algae and invertebrates are 19.0 and 19.5 mg/L, respectively, for the free acid form of TPA. Both values exceed the trigger value of 0.01 mg/L.

Based on available data, classification criteria are not met.

CAS: 100-21-0 terephthalic acid

ErC50/72h	668 mg TPA equiv/L (Desmodesmus subspicatus) (OECD Guideline 201 (Alga, Growth Inhibition test))
LC50/96 h	>18.6 mg TPA equiv/L (Oryzias latipes) (OECD Guideline 203 (Fish, Acute))
LC50/96 h (static)	> 961 mg TPA equiv/L (Leuciscus idus) (OECD Guideline 203)
EC50/48h (static)	>967 mg TPA equiv//L (Daphnia sp.) (OECD Guideline)
EC50/72h	>19 mg/L (Pseudokirchneriella subcapitata) (OECD Guideline 201)
NOEC/21d	>19.5 mg/L (Daphnia sp.) (OECD Guideline 211)

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- **12.2 Persistence and degradability**

Readily biodegradable.

Terephthalic acid is readily biodegradable and therefore does not satisfy the criteria for classification as persistent (P). (CITI, 1975); (Lebertz, 1991a).

- **12.3 Bioaccumulative potential**

Terephthalic acid has low potential for bioaccumulation (e. g., log Kow < 3) and does not satisfy the criterion for classification as bioaccumulative (B).

- **12.4 Mobility in soil**

Adsorption to solid phase is possible.

The predicted log Kow value for terephthalic acid is 2.00 (KOWWIN database, 2008)

- **12.5 Results of PBT and vPvB assessment**

- **PBT:** The substance does not meet the PBT criteria (not PBT) according to (EC) 1907/2006, Annex XIII.

- **vPvB:** The substance does not meet the vPvB criteria (not vPvB) according to (EC) 1907/2006, Annex XIII.

- **12.6 Endocrine disrupting properties** The product does not contain substances with endocrine disrupting properties.

- **12.7 Other adverse effects** No further relevant information available.

- **Additional ecological information:**

- **General notes:**

Water hazard class 1 (German Regulation) (Self-assessment): slightly hazardous for water.

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

SECTION 13: Disposal considerations

- **13.1 Waste treatment methods**

- **Recommendation**

Vacuum or sweep up material and place in a designated labelled waste container.

Dispose of via a licensed waste disposal contractor.

- **Uncleaned packaging:**

- **Recommendation:** Disposal must be made according to official regulations.

- **Recommended cleansing agents:** Water, if necessary together with cleansing agents.

SECTION 14: Transport information

- **14.1 UN number or ID number**

- **ADR, ADN, IMDG, IATA** not applicable

- **14.2 UN proper shipping name**

- **ADR, ADN, IMDG, IATA** not applicable

- **14.3 Transport hazard class(es)**

- **ADR, ADN, IMDG, IATA**

- **Class** not applicable

- **14.4 Packing group**

- **ADR, IMDG, IATA** not applicable

- **14.5 Environmental hazards:**

- **Marine pollutant:** No

- **14.6 Special precautions for user**

Not applicable.

- **14.7 Maritime transport in bulk according to IMO instruments**

Not applicable.

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· UN "Model Regulation": not applicable

SECTION 15: Regulatory information

- **15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture --**
- **Inventory - United States - Toxic Substances Control Act (TSCA) ACTIVE**
- **OECD - List of High Production Volume Chemicals** Substance is not listed.
- **Inventory - Canada - Domestic Substances List (DSL)** Substance is listed
- **Philippines Inventory of Chemicals and Chemical Substances** Substance is listed.
- **Chinese Chemical Inventory of Existing Chemical Substances (IECSC)** Substance is listed.
- **Australian Inventory of Industrial Chemicals** Substance is listed.
- **Inventory - Korea - Existing and Evaluated Chemical Substances KE-02190**
- **New Zealand Inventory of Chemicals** Substance is listed.
- **Japan Existing and New Chemical Substances (ENCS) 3-1334**
- **DIRECTIVE 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment – Annex II**
Substance is not listed.
- **REGULATION (EU) 2019/1148**
- **Annex I - RESTRICTED EXPLOSIVES PRECURSORS (Upper limit value for the purpose of licensing under Article 5(3))**
Substance is not listed.
- **Annex II - REPORTABLE EXPLOSIVES PRECURSORS** Substance is not listed.
- **15.2 Chemical safety assessment:** A Chemical Safety Assessment has been carried out.

SECTION 16: Other information

A Chemical Safety Assessment has been carried out.

- **Exposure scenarios**
This substance is not classified for human health or the environment, is not a CMR and is not PBT or vPvB. Therefore, it is not required the development of exposure scenarios.
- **Version number of previous version:** 2
- **Abbreviations and acronyms:**
RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
ICAO: International Civil Aviation Organisation
NOAEL: Non Observed Adverse Effect Level
LOAEL: Lowest Observed Adverse Effect Level
ADR: Accord relatif au transport international des marchandises dangereuses par route (European Agreement Concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
IATA: International Air Transport Association
GHS: Globally Harmonised System of Classification and Labelling of Chemicals
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
DNEL: Derived No-Effect Level (REACH)
PNEC: Predicted No-Effect Concentration (REACH)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
PBT: Persistent, Bioaccumulative and Toxic
vPvB: very Persistent and very Bioaccumulative
- *** Data compared to the previous version altered.**
Version 1 Revision 25.05.2011
Version 2 Revision 04.11.2011
Change of Only Representative.
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General review.
Update of the address of the Only Representative.
Updated contact e-mail.

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EU

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Annex: Exposure scenario

· **Short title of the exposure scenario** Empty section of the SDS: not required.

EU