

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Terephthalic acid for synthesis

Revision date: 19.11.2024

Product code: 19913

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

1.1. Product identifier

Terephthalic acid for synthesis

REACH Registration Number: 01-2119485970-27-XXXX
CAS No: 100-21-0
EC No: 202-830-0

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

Use of the substance/mixture

Laboratory chemical

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name: AnalytiChem GmbH
ACD
Street: Stempelstraße 6
Place: D-47167 Duisburg
Telephone: 0203/5194-0
Telefax: 0203/5194-290
E-mail: info@analytichem.de
Contact person: Abteilung Produktsicherheit
Telephone: 0203/5194-107/117
E-mail: produktsicherheit@analytichem.de
Internet: www.analytichem.de
Responsible Department: Abteilung Produktsicherheit

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

This substance is not classified as hazardous in accordance with Regulation (EC) No 1272/2008.

2.2. Label elements

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C₈H₆O₄
Molecular weight: 166,13 g/mol

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Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
100-21-0	terephthalic acid			100 %
	202-830-0		01-2119485970-27-XXXX	

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
100-21-0	202-830-0	terephthalic acid	100 %
	dermal: LD50 = > 2000 mg/kg; oral: LD50 = > 15380 mg/kg		

Further Information

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

No data available

After inhalation

Provide fresh air.

Call a doctor if you feel unwell.

After contact with skin

Wash immediately with: Water

Take off immediately all contaminated clothing and wash it before reuse.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water.

In case of eye irritation consult an ophthalmologist.

After ingestion

Rinse mouth immediately and drink plenty of water.

Call a doctor if you feel unwell.

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

No data available

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

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings.

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible solids

Hazardous combustion products

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Danger of dust explosion.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

Additional information

Suppress gases/vapours/mists with water spray jet.

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Provide adequate ventilation.

Use personal protection equipment.

Avoid contact with skin, eyes and clothes.

Remove persons to safety.

Emergency procedures

Consult an expert

Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

For containment

Cover drains.

Prevent spread over a wide area (e.g. by containment or oil barriers).

Collect in closed and suitable containers for disposal.

Take up carefully when dry. Take up dust-free and set down dust-free.

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

Provide adequate ventilation.

Do not breathe dust/fume/gas/mist/vapours/spray.

Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Avoid dust formation.

Do not breathe dust.

Advice on protection against fire and explosion

Danger of dust explosion.

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Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.
Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink.

Further information on handling

Wash hands and face before breaks and after work and take a shower if necessary.
Take off immediately all contaminated clothing and wash it before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed.
Store in a dry place.

Further information on storage conditions

storage temperature: +15°C - +25°C

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Occupational exposure limits

CAS No	Substance	ppm	mg/m ³	fib/cm ³	Category	Origin
100-21-0	Terephthalic acid	-	10		TWA (8 h)	

DNEL/DMEL values

CAS No	Substance			
DNEL type		Exposure route	Effect	Value
100-21-0	terephthalic acid			
Worker DNEL, long-term		dermal	systemic	21 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	4 mg/m³
Consumer DNEL, long-term		dermal	systemic	11 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	1,25 mg/kg bw/day
Worker DNEL, long-term		inhalation	systemic	15 mg/m³

PNEC values

CAS No	Substance	
Environmental compartment		Value
100-21-0	terephthalic acid	
Freshwater		0,38 mg/l
Freshwater (intermittent releases)		1,9 mg/l
Marine water		0,038 mg/l
Freshwater sediment		0,52 mg/kg
Micro-organisms in sewage treatment plants (STP)		50 mg/l
Soil		0,71 mg/kg

8.2. Exposure controls

Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection

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equipment.

Individual protection measures, such as personal protective equipment

Eye/face protection

Suitable eye protection: goggles.

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact

Trade name/designation: KCL 741 Dermatril® L

Recommended material: NBR (Nitrile rubber) 0,11 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation: KCL 741 Dermatril® L

Recommended material: NBR (Nitrile rubber) 0,11 mm

Wearing time with occasional contact (splashes): > 480 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. This recommendation applies only to the product stated in the safety data sheet<(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Skin protection

Wear suitable protective clothing.

The choice of body protection depends on the concentration and quantity of hazardous substances. The chemical resistance of protective agents must be clarified with their suppliers.

Respiratory protection

Respiratory protection necessary at: dust formation

Filtering device with filter or ventilator filtering device of type: P1

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not allow to enter into surface water or drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	solid
Colour:	white
Odour:	characteristic
Melting point/freezing point:	402 °C
Boiling point or initial boiling point and boiling range:	No data available
Flammability:	No data available
Lower explosion limits:	No data available

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Upper explosion limits:	No data available
Flash point:	No data available
Auto-ignition temperature:	496 °C
Decomposition temperature:	No data available
pH-Value:	No data available
Viscosity / kinematic:	No data available
Water solubility: (at 20 °C)	0,015 g/l
Solubility in other solvents	No data available
Partition coefficient n-octanol/water:	log Pow: 1,76
Vapour pressure:	No data available
Vapour pressure:	No data available
Density (at 20 °C):	1,51 g/cm ³
Bulk density:	No data available
Relative vapour density:	No data available

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

Danger of dust explosion.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Sustaining combustion:

No data available

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

Not oxidising.

Other safety characteristics

Evaporation rate:

No data available

Solvent separation test:

No data available

Solvent content:

No data available

Solid content:

No data available

Sublimation point:

No data available

Softening point:

No data available

Pour point:

No data available

No data available:

Viscosity / dynamic:

No data available

Flow time:

No data available

Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Danger of dust explosion.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

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Violent reaction with:
Oxidising agent, strong

10.4. Conditions to avoid

No data available

10.5. Incompatible materials

No data available

10.6. Hazardous decomposition products

No data available

Further information

No data available

SECTION 11: Toxicological information

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

Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

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

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
100-21-0	terephthalic acid				
	oral	LD50 mg/kg > 15380	Rat	Other company data (1975)	OECD Guideline 401
	dermal	LD50 mg/kg > 2000	Rabbit	Study report (1990)	OECD Guideline 402

Irritation and corrosivity

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

Serious eye damage/eye irritation: Based on available data, the classification criteria are not met.

slightly irritant but not relevant for classification.

Sensitising effects

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

Carcinogenic/mutagenic/toxic effects for reproduction

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

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

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

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.

Aspiration hazard

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

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards

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Other information

No data available

Further information

Cough

Dyspnoea

SECTION 12: Ecological information

12.1. Toxicity

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

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
100-21-0	terephthalic acid					
	Acute fish toxicity	LC50 mg/l	> 961	96 h	Leuciscus idus melanotus	Study report (1993) OECD Guideline 203
	Acute algae toxicity	ErC50 mg/l	> 19	72 h	Pseudokirchneriella subcapitata	Study report (2003) OECD Guideline 201
	Acute crustacea toxicity	EC50 mg/l	> 967	48 h	Daphnia magna	Study report (1993) OECD Guideline 202
	Crustacea toxicity	NOEC mg/l	19,5	21 d	Daphnia magna	Study report (2003) OECD Guideline 211

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No indication of bioaccumulation potential.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
100-21-0	terephthalic acid	1,76

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

Discharge into the environment must be avoided.

Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.

Do not empty into drains.

Contaminated packaging

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

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SECTION 14: Transport information

Land transport (ADR/RID)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Inland waterways transport (ADN)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Marine transport (IMDG)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Air transport (ICAO-TI/IATA-DGR)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No dangerous good in sense of this transport regulation.

14.7. Maritime transport in bulk according to IMO instruments

not applicable

SECTION 15: Regulatory information

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

EU regulatory information

Information according to Directive 2012/18/EU (SEVESO III): Not subject to 2012/18/EU (SEVESO III)

National regulatory information

Water hazard class (D): 1 - slightly hazardous to water

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 12.

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Abbreviations and acronyms

ADR: Accord européen sur le transport 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 Harmonized System of Classification and Labelling of Chemicals
EINECS: European Inventory of Existing Commercial Chemical Substances
ELINCS: European List of Notified Chemical Substances
CAS: Chemical Abstracts Service
LC50: Lethal concentration, 50%
LD50: Lethal dose, 50%

Further Information

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material. The receiver of our product is singularly responsible for adhering to existing laws and regulations. Provide appropriate information, instructions and training to users