



POLIEF JSC

SAFETY DATA SHEET

According to EC Regulations 1907/2006 (REACH), 1272/2008 (CLP) & 453/2010

TEREPHTHALIC ACID

VERSION: 2.2
DATE CREATED: 01/07/2013

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND COMPANY/UNDERTAKING

1.1 Product identifier

NAME OF SUBSTANCE:	Terephthalic acid
SYNONYMS:	P-Benzenedicarboxylic acid; 1,4-Benzenedicarboxylic acid
TRADE NAMES:	Terephthalic acid
Index No (CLP)	none
CAS #:	100-21-0
EC #:	202-830-0
REGISTRATION #:	01-2119485970-27-0018

1.2. Relevant identified uses of the substance. See Annex 1

Most common technical function of substance:

Intermediates

Laboratory chemicals

Uses advised against

The use of the substance should be limited to those specified in Annex 1.

1.3. Details of the supplier of the safety data sheet

Only representative	
Company name:	Gazprom Marketing and Trading France
Address:	68 avenue des Champs-Élysées, 75008, Paris, France
Contact Telephone:	+33 1 42 99 73 50
Fax:	+33 1 42 99 73 99
Email Address:	Yury.severinchik@gazprom-mt.com

Suppliers	
Company name:	POLIEF JSC
Address:	Socialisticheskaya str.71, Blagoveschensk, 453434, Republic of Bashkortostan
Phone:	+7 3472 79-73-20; 79-75-46
Fax:	+7 3472 52-35-41
Email Address:	polyef@polyef.ru
Emergency phone:	+7 3472 52-35-41 (9.00 to 18.00, GMT+5)



1.4 Emergency phone in the country of delivery:	112 (Please note that emergency numbers may vary depending upon the country of delivery though 112 remains valid as universal number)
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SECTION 2. HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

2.1.1 Classification according to Directive 67/548/EEC
Not classified as a dangerous substance.

2.1.2 Classification according to Regulation (EC) No 1272/2008 (CLP/GHS)
Not classified as a hazardous substance.

2.2 Label elements

2.2.1 Labelling according to Regulation (EC) No 1272/2008 (CLP/GHS)
Not applicable.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Name	EC #	CAS #	Content, %	Classification EC#67/548/EEC and EC#1272/2008 (CLP)
Terephthalic acid	202-830-0	100-21-0	≥99.6%	none

Specific Conc. Limits (CLP): none.
M-factor: none.

The product does not contain impurities or additives that could affect product's labelling and classification according to Regulation (EC) No 67/548/EEC and Regulation (EC) No 1272/2008 (CLP) in the concentration ranges specified.

SECTION 4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation:

If inhaled, remove to fresh air. Get medical attention if symptoms appear.

Ingestion:

Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately.

Skin contact:

Wash exposed skin with soap and water.
Get medical attention if irritation develops.



Eye contact:

In case of contact, flush eyes immediately with copious amounts of water for at least 15 minutes. Get medical attention if irritation occurs.

SECTION 5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media:

Suitable extinguishing media includes water spray (fog), foam, dry chemical or CO2 extinguisher or spray.

Unsuitable fire extinguishing media includes water jet.

5.2 Special fire-fighting procedures:

None identified.

5.3 Unusual fire/explosion hazards:

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.

5.4 Hazardous decomposition products:

Decomposition products may include the following materials - carbon dioxides.

5.5 Protection of fire-fighters:

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:

No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.

See section 8.

6.2 Environmental precautions:

Avoid breathing dust. Avoid creating dusty conditions and prevent wind dispersal. Eliminate all ignition sources if safe to do so. 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 Large spill:

Move containers from spill area. Approach the release from upwind. 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 Small spill:

Move containers from spill area. Vacuum or sweep up material and place in a designated labelled waste container. Dispose of via a licensed waste disposal contractor.



SECTION 7. HANDLING AND STORAGE

7.1 Handling:

Avoid breathing dust. Keep away from heat, sparks and flame. To avoid fire or explosion, dissipate static electricity during transfer by earthing and bonding containers and equipment before transferring material. Take precautionary measures against static electricity. The need for additional measures for explosion protection should be evaluated (see NFPA 68--Guide for Venting of Deflagrations; and NFPA 69--Standard on Explosion Prevention Systems). Wash thoroughly after handling.

7.2 Storage:

Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

8.1.1 Occupational Exposure Limits:

International Limit Values¹⁾

SUBSTANCE Terephthalic acid CAS #100-21-0	LTEL 8 hr TWA ppm	LTEL 8 hr TWA mg/m ³	STEL ppm	STEL mg/m ³	Note
Belgium		10			
Denmark		10		20	
European Union	-	-	-	-	
Germany (DFG)		5 inhalable aerosol		10 inhalable aerosol (1)	(1) 15 minutes average value
Spain		10			
Switzerland		5 inhalable aerosol		10 inhalable aerosol (1)	
USA - NIOSH	-	-	-	-	
USA - OSHA	-	-	-	-	

¹⁾ GESTIS International Limit values:
http://limitvalue.ifa.dguv.de/WebForm_ueliste.aspx

8.1.2 DNEL/ PNEC values:

DN(M)ELs for workers

Exposure pattern	Route	Descriptors	DNEL/ DMEL (appropriate unit)	Justification
Long-term - systemic effects	Dermal	DNEL (Derived No Effect Level)	67 mg/kg bw/d	



Long-term - systemic effects	Inhalation	DNEL (Derived No Effect Level)	23 mg/m³	
Acute - systemic effects	Dermal	No-threshold effect and/or no dose-response information available	-	In the absence of acute systemic toxicity, no dose-response data are available and a quantitative dose descriptor is not derived. DNEL values for acute dermal systemic effects are therefore not calculated.
Acute - systemic effects	Inhalation	No-threshold effect and/or no dose-response information available	-	
Acute - local effects	Dermal	No-threshold effect and/or no dose-response information available	-	In the absence of local effects following short-term or long-term exposure, no dose-response data are available and a quantitative dose descriptor is not derived. DNEL values for local exposure are therefore not calculated.
Acute - local effects	Inhalation	No-threshold effect and/or no dose-response information available	-	
Long-term - local effects	Dermal	No-threshold effect and/or no dose-response information available	-	
Long-term - local effects	Inhalation	No-threshold effect and/or no dose-response information available	-	

DN(M)ELs for the general population

Exposure pattern	Route	Descriptors	DNEL/ DMEL (appropriate unit)	Justification
Long-term - systemic effects	Dermal	DNEL (Derived No Effect Level)	33 mg/kg bw/d	
Long-term - systemic effects	Inhalation	DNEL (Derived No Effect Level)	5.8 mg/m ³	
Long-term - systemic effects	Oral	DNEL (Derived No Effect Level)	3.3 mg/kg bw/d	
Acute - systemic effects	Dermal	No-threshold effect and/or no dose-response information available	-	In the absence of acute systemic toxicity, no dose-response data are available and a quantitative dose descriptor is not derived. DNEL values for acute systemic effects are therefore not calculated.
Acute - systemic effects	Inhalation	No-threshold effect and/or no dose-response information available	-	



Acute - systemic effects	Oral	No-threshold effect and/or no dose-response information available	-	In the absence of local effects following short-term or long-term exposure, no dose-response data are available and a quantitative dose descriptor is not derived. DNEL values for local exposure are therefore not calculated.
Acute - local effects	Dermal	No-threshold effect and/or no dose-response information available	-	
Acute - local effects	Inhalation	No-threshold effect and/or no dose-response information available	-	
Long-term - local effects	Dermal	No-threshold effect and/or no dose-response information available	-	
Long-term - local effects	Inhalation	No-threshold effect and/or no dose-response information available	-	

PNEC water	Value	Assessment factor
PNEC aqua – freshwater (mg/l)	0.38 mg/L	50
PNEC aqua - marine water (mg/l)	0.038 mg/L	500
PNEC aqua – intermittent releases (mg/l)	1.9 mg/L	10

PNEC sediment	Value	Assessment factor
PNEC sediment freshwater	0.52 mg/kg sediment dw	
PNEC sediment (marine water):	0.052 mg/kg sediment dw	

PNEC soil	Value	Assessment factor
PNEC soil (mg/kg soil dw)	PNEC soil: 0.71 mg/kg soil dw	

PNEC sewage treatment plant	Value	Assessment factor
PNEC STP (mg/l.)	PNEC STP: 50 mg/L	10

Calculation of PNECoral (secondary poisoning)	Value	Assessment factor
PNEC oral (mg/kg food)	No potential for bioaccumulation	



8.2 Exposure controls:

8.2.2 Occupational exposure controls:

Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

8.2.3 Hygiene measures:

Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period.

8.2.4 Personal protective equipment

Respiratory protection:

If dust is generated and ventilation is inadequate, use a respirator that will protect against dust/mist. If concentration is unknown, a Self-Contained Breathing Apparatus (SCBA) should be used to avoid inhalation of the product.

Hand protection:

The correct choice of protective gloves depends upon the chemicals being handled, the conditions of work and use, and the condition of the gloves. Most gloves provide only a short time of protection before they must be discarded and replaced. Because specific work environments and material handling practices vary, safety procedures should be developed for each intended application. Gloves should therefore be chosen in consultation with the supplier/manufacturer and with a full assessment of the working conditions.

Eye protection:

Avoid contact with eyes. Use chemical/dust goggles.

Skin and body:

None required; however, use of protective clothing is good industrial practice.

8.2.5. Environmental Exposure Controls:

None specific.

Do not allow penetration of the product into water reservoirs, surface and ground water, sewer ducts and soil.

Preventing disposal into water reservoirs of contaminated water without treatment.

Content of dust in the air should be monitored.

Provide sealing of process equipment.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Property	Value	Remarks
Physical state at 20°C and 101.3 kPa	Terephthalic acid is an organic substance commercially available as a white, free-flowing, crystalline powder. The commercial production process typically results in the formation of rounded crystals. Needles may be formed by slow crystallisation, but may	



Property	Value	Remarks
	alter flow characteristics.	
Melting/freezing point	Terephthalic acid sublimates at 402 - 404 °C at atmospheric pressure. Under normal conditions TPA will therefore undergo direct transition from the solid to the vapour phase without melting. Melting has been observed to occur at 427°C under sealed tube conditions.	
Boiling point	Terephthalic acid is a solid. It sublimates at 402-404 °C at atmospheric pressure, without undergoing a transition to the liquid phase. Its boiling point cannot therefore be determined except under artificial physical conditions that have no practical relevance.	
Relative density	The crystal density of Terephthalic acid is 1.58 g/cm ³ at 25 °C. The specific gravity of Terephthalic acid is 1.522 at 25 °C.	
Particle size distribution (granulometry)	The particle size distribution was characterised by the Coulter method as follows: particles of diameter <4, <10 and <100 microns comprised 0.66%, 1.16% and 38.86%, respectively, of the sample by volume and 61.14% of the sample consisted of particles with a diameter >100 microns.	The data provided by the Lead Registrant are compatible with other, independently collated data contributed by members of the Terephthalic Acid Sub-Group of the Polyester Monomers Consortium (contributors anonymised, number of sources not known), whose collective particle size distribution data are described by the following envelope: 15% to 30% smaller than 50 microns, 75% to 90% in the range 40 to 350 microns.
Vapour pressure	0.00158 Pa at 25 °C The vapour pressure estimate for Terephthalic acid is very low, compared to standard atmospheric pressure and TPA is therefore not likely to volatilise to the atmosphere.	The vapour pressure of Terephthalic acid was estimated using the QSAR model MPBPVP v.1.43 of the US EPA. The definitive value calculated according to the Modified Grain method. Based on a mathematical relationship between temperature and vapour pressure for TPA, derived from published VP measurements at temperatures in the range 100 to 250 °C, the vapour pressure of TPA at 25°C is estimated to be 0.000000000259 mm Hg.
Surface tension	No data is available: a waiver is proposed. Terephthalic acid has no application in detergency and surface activity is not a desired function in any of its uses. Consequently, a test of the surface tension of Terephthalic acid in	In accordance with Column 2 adaptation statement of REACH Annex VII, information requirement 7.6, this study does not need to be conducted if, based on structure, surface activity is not expected and no surface-active

Property	Value	Remarks
	aqueous solution is not required.	properties would be predicted for this compound. Surface activity is not a desired property of the material
Water solubility	17 mg/L at 25 °C	The limit of solubility of Terephthalic acid (TPA) in water at 25 °C is <i>ca.</i> 17 to 19 mg/L. TPA is therefore considered to be slightly soluble in water.
Partition coefficient n-octanol/water (log value)	Log Kow (Pow): 2 at 25 °C	
Flash point	No data is available: a waiver is proposed and an experimental flashpoint determination is not required	In accordance with Section 2 of REACH Annex XI, information requirement section 7.9, this study does not need to be conducted based on the physical state of the molecule. According to ECHA guidance, flash point is only relevant to liquids and low melting point solids
Flammability	non flammable	A preliminary flammability screening test was performed by igniting a loosely-packed linear pile of TPA. Combustion self-extinguished after 218 seconds and without propagating 200 mm along the pile. According to the UN Recommendations on the Transport of Dangerous Goods, Terephthalic acid is therefore not classified as a readily combustible solid of Division 4.1 and further flammability testing is not required.
Explosive properties	non explosive	According to theoretical considerations based on chemical structure, Terephthalic acid does not possess explosive or oxidising properties. Terephthalic acid is unlikely to undergo rapid decomposition accompanied by the evolution of gases or release of heat and therefore does not present a risk of explosion.
Self-ignition temperature	No data is available: a waiver is proposed. In the absence of self-heating at 400 °C an experimental determination of auto-flammability is not required.	Terephthalic acid is a solid that sublimates at 402-404 °C at atmospheric pressure, without evidence of self-heating. In the absence of self-heating at 400 °C an experimental determination of auto-flammability (the lowest temperature at which Terephthalic acid will spontaneously ignite in the absence of an external ignition source) is not required.
Oxidising	Oxidising: no	According to theoretical considerations based on chemical structure,



Property	Value	Remarks
properties		Terephthalic acid does not possess oxidising properties. Terephthalic acid is unlikely to cause or contribute to the combustion of other material during transport, storage or use.
Stability in organic solvents and identity of relevant degradation products	No data is available: a waiver is proposed as it is not expected that the stability of Terephthalic acid in organic solvents is critical.	In accordance with REACH Annex XI Section 2, with reference to the guidance mentioned in REACH Art 13(3) the test guidance "ECHA guidance on information requirements and chemical safety assessment Chapter R.7a Endpoint Specific Guidance"; this study does not need to be conducted since the stability in organic solvents is not considered critical. This would be assessed in individual studies where organic solvents are used.
Dissociation constant	The pK1 and pK2 values for Terephthalic acid in aqueous solution at 25 °C are 3.54 and 4.46, respectively.	
Viscosity	No data is available: a waiver is proposed as Terephthalic acid is a solid under standard conditions.	In accordance with Section 2 of REACH Annex XI, information requirement section 7.17, this study cannot be conducted on solid materials or gases. According to ECHA Chapter 7 guidance, viscosity measurement is only relevant to liquids.

SECTION 10. STABILITY AND REACTIVITY

10.1 Stability:

The product is stable. Under normal conditions of storage and use, hazardous polymerization will not occur.

10.2 Conditions to avoid:

Keep away from heat, sparks and flame. Take precautionary measures against static discharges.

10.3 Hazardous decomposition products:

Combustion products may include the following - carbon oxides. Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11. TOXICOLOGICAL INFORMATION

Property	Value / Remarks
Acute toxicity: Acute oral toxicity	LD50 (oral): 15380 mg/kg bw
Acute inhalation toxicity	LC50 (inhalation): 1000 mg/m ³ air
Acute dermal toxicity	

	LD50 (dermal): 2000 mg/kg bw
Skin irritation/corrosion	not irritating
Skin sensitisation	not sensitising
Eye irritation	not irritating
Respiratory irritation/ sensitisation	Not irritating/ not sensitising
Repeated dose toxicity	Route: oral: NOAEL: 125 mg/kg bw/d (sub-chronic; rat) Route: inhalation: NOAEC: 10 mg/m ³
Toxicokinetics: <u>Basic toxicokinetics</u>	No bioaccumulation potential. Terephthalic acid is rapidly absorbed and is rapidly excreted predominantly in the urine as the sulphate conjugate. The weight of evidence indicates that there is little potential for bioaccumulation (<i>oral administration</i>).
<u>Dermal absorption</u>	No significant dermal absorption is reported in the rat following a single or repeated dermal application of 80 mg of radiolabelled TPA. Absorption rate (%): 10
Mutagenicity:	Genetic toxicity: negative No evidence of genotoxicity was seen in an Ames test. Data from in vitro clastogenicity studies are equivocal; however there are clearly negative studies in vivo.
Carcinogenicity:	No classification is proposed for carcinogenicity. LOAEL: 1000 mg/kg bw/d (Route: oral. Target organs: urogenital: urinary bladder). Data indicate that the chronic administration of terephthalic acid at high concentrations results in the formation of urinary bladder tumours as a consequence of chronic inflammation secondary to calculus formation. Findings were only seen at dose levels that will not be encountered by humans following occupational exposure and, additionally, rats are known to be more susceptible to urolithiasis. TPA is non-genotoxic and the carcinogenicity seen in rats is a threshold effect associated with chronic mechanical irritation.
Toxicity for reproduction:	No evidence of reproductive toxicity was seen in a modern two-generation study. NOAEL (route: oral): 2010.9 mg/kg bw/d
Developmental toxicity:	No evidence of developmental toxicity was seen in an inhalation study in rats NOAEC (route: inhalation): 10 mg/m ³

SECTION 12. ECOLOGICAL INFORMATION

Property	Value / Remarks
Ecotoxicity:	
Aquatic toxicity:	<p>96 -h LC₅₀ (static): >961 mg TPA-equiv/L, 96 -h NOEC: 961 mg TPA-equiv/L.</p> <p>Terephthalic acid and its more environmentally relevant terephthalate sodium salt exhibit very low short-term toxicity to fish.</p>
Long term toxicity testing on invertebrates (calculated):	<p>Not available.</p> <p>In accordance with Column 2 of REACH Annex IX, the study does not need to be conducted as all identified uses of the substance are assessed as safe for the environment.</p> <p>This data point has been waived for Terephthalic acid on the grounds that exposure is not expected to occur and that TPA is readily biodegradable and therefore non-persistent. Under these circumstances, data for the long-term effects of Terephthalic acid on fish and the concomitant expenditure of vertebrate test organisms are considered unnecessary.</p>
Toxicity to Algae and aquatic plants (<i>P. subcapitata</i>)	<p>EC₁₀/LC₁₀ or NOEC for freshwater algae: 19 mg/L</p> <p>Terephthalic acid and its more environmentally relevant terephthalate sodium salt exhibit very low toxicity to unicellular aquatic algae.</p>
Short term toxicity testing on fish (<i>D. magna</i>)	<p>48 -h EC₅₀ (static): >967 mg TPA-equiv/L; 96 -h NOEC: 967 mg TPA-equiv/L</p> <p>Terephthalic acid and its more environmentally relevant terephthalate sodium salt exhibit very low short-term toxicity to aquatic invertebrates</p>
Long term toxicity testing on fish (<i>D. magna</i>)	<p>21 -d NOEC (semi-static): 19.5 mg TPA/L.</p> <p>This endpoint is a mean measured value and represents the maximum limit concentration achievable under the test conditions.</p> <p>Terephthalic acid exhibits low long-term toxicity to aquatic invertebrates.</p>
Toxicity to sediment organisms:	<p>Not available.</p> <p>In accordance with Column 2 of REACH Annex IX, the study does not need to be conducted as all identified uses of the substance are assessed as safe for the environment.</p> <p>This data point has been waived for Terephthalic acid on the grounds that exposure is not expected to occur and that TPA</p>



Property	Value / Remarks
	<p>is readily biodegradable and has no strong tendency to partition toward organic matter in sediment. Under these circumstances, data for the effects of Terephthalic acid on sediment-dwelling organisms are considered unnecessary.</p>
Terrestrial toxicity:	
<p>Toxicity to soil macro-organisms:</p>	<p>No data are available on the toxicity of Terephthalic acid to soil macroorganisms.</p> <p>This data point has been waived for Terephthalic acid on the grounds that exposure is not expected to occur and that TPA is readily biodegradable. Under these circumstances, data for the effects of Terephthalic acid on soil macroorganisms are considered unnecessary</p>
<p>Toxicity on soil soil arthropods:</p>	<p>No data are available on the toxicity of Terephthalic acid to terrestrial arthropods.</p> <p>This data point has been waived for Terephthalic acid on the grounds that exposure is not expected to occur and that TPA is readily biodegradable. Under these circumstances, data for the effects of Terephthalic acid on terrestrial arthropods are considered unnecessary.</p>
<p>Toxicity to terrestrial plants</p>	<p>No data are available on the toxicity of Terephthalic acid to terrestrial plants/</p> <p>This data point has been waived for Terephthalic acid on the grounds that exposure is not expected to occur and that TPA is readily biodegradable. Under these circumstances, data for the effects of Terephthalic acid on terrestrial plants are considered unnecessary.</p>
<p>Toxicity on soil microorganism:</p>	<p>No data are available on the toxicity of Terephthalic acid to soil microorganisms.</p> <p>This data point has been waived for Terephthalic acid on the grounds that exposure is not expected to occur and that TPA is readily biodegradable. Under these circumstances, data for the effects of Terephthalic acid on soil microorganisms are considered unnecessary.</p>

Property	Value / Remarks
Toxicity to mammals	<p>No data are available on the toxicity of Terephthalic acid to other above-ground organisms.</p> <p>This data point has been waived for Terephthalic acid on the grounds that contamination of the terrestrial compartment is unlikely, that TPA is readily biodegradable and that primary exposure of terrestrial vertebrates is therefore not expected to occur. Moreover, the log Kow of Terephthalic acid is less than 3.0, indicating that its bioconcentration potential is negligible and there is consequently no significant risk of secondary poisoning of other above-ground organisms via earthworms or fish. Under these circumstances, data for the effects of Terephthalic acid on other above-ground organisms are considered unnecessary.</p>
Long-term or reproductive toxicity to birds:	<p>No data are available on the toxicity of Terephthalic acid to birds.</p> <p>This data point has been waived for Terephthalic acid on the grounds that contamination of the terrestrial compartment is unlikely, that TPA is readily biodegradable and that primary exposure of terrestrial vertebrates is therefore not expected to occur. Moreover, the log Kow of Terephthalic acid is less than 3.0, indicating that its bioconcentration potential is negligible and there is consequently no significant risk of secondary poisoning of birds via earthworms or fish. Under these circumstances, data for the effects of Terephthalic acid on birds are considered unnecessary.</p>
Adsorption / desorption:	<p>In accordance with Column 2 adaptation statement of REACH Annex VIII and IX, adsorption/desorption screening and further studies on adsorption/desorption, information requirements 9.3.1 and 9.3.3, may be omitted since the log Kow value for the substance is <3.0 and has low potential for adsorption (CSR section 1.3).</p> <p>(Q)SAR-modelled Koc values for Terephthalic acid range from 18.28 to 79.24 L/kg.</p>
Biotic degradation:	<p>The test results show that TPA is biodegradable under anaerobic, methanogenic conditions and it may be inferred that Terephthalic acid is also likely to be degraded in other anaerobic environments, such as water-logged soils or sediments.</p> <p>Terephthalic acid is not persistent (not P).</p> <p>Based on its physico-chemical properties, Terephthalic acid is expected to partition mainly toward the aqueous compartment during wastewater treatment and to be channelled predominantly toward aerobic biological (e.g. activated sludge) treatment. Nevertheless, a significant (albeit minor) proportion may become associated with sludge solids during primary settlement or with waste</p>



Property	Value / Remarks
	activated sludge and be directed toward thermophilic anaerobic digestion, which typically precedes the disposal of wastewater treatment sludges to land or alternatively by land-filling or incineration
Abiotic degradation:	<p>Not available.</p> <p>In accordance with Column 2 adaptation statement of REACH Annex VIII, hydrolysis as a function of pH, information requirement 9.2.2.1, does not need to be conducted if the test substance is readily biodegradable</p> <p>Terephthalic acid is generally resistant to physico-chemical degradation processes under the range of conditions likely to be encountered in the aquatic and terrestrial environment.</p>
Biodegradation in water and sediment:	<p>In accordance with REACH Annex IX column 2, simulation tests of biodegradation in water and sediment are not required because Terephthalic acid is readily biodegradable</p> <p>74.7% degradation of TPA dosed at 100 mg/L was recorded in 14 days by the principal indicator of mineralisation based on oxygen uptake measurements.</p> <p>HPLC and UV-VIS spectrometric analyses showed 99.3% and 100% loss of the parent substance, respectively, during the 14-d incubation.</p>
Biodegradation in soil	In accordance with REACH Annex IX Column 2, tests of biodegradation in soil are not required because Terephthalic acid is readily biodegradable.
Simulation testing:	<p>In accordance with Column 2 adaptation statement of REACH Annex IX, simulation testing on ultimate degradation in surface water, information requirement 9.2.1.2, does not need to be conducted given the test substance is readily biodegradable.</p> <p>In accordance with Column 2 adaptation statement of REACH Annex IX, sediment simulation testing, information requirement 9.2.1.4, does not need to be conducted given the substance is readily biodegradable.</p>
<p>Phototransformation/photolysis:</p> <p><u>Phototransformation in air</u></p> <p><u>Phototransformation in water</u></p>	<p>Half-life in air: 13 d (AOPWIN v1.91 QSAR model available from the US EPA.)</p> <p>Not available.</p> <p>Studies of photolysis in water are not necessary for Terephthalic acid.</p> <p>Under environmental conditions, photolysis is unlikely to make a significant contribution to the dissipation of Terephthalic acid (or its salts), compared to the rate of its removal by biodegradation.</p>
Aquatic/ Terrestrial bioaccumulation	In accordance with Column 2 adaptation statement of



Property	Value / Remarks
	REACH Annex IX, information requirement section 9.3.2, a bioaccumulation study need not be conducted if the substance has low potential for bioaccumulation (e. g., log Kow < 3).
<u>PBT/vPvB</u>	Terephthalic acid is neither a PBT nor a vPvB substance.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal considerations / Waste information:

The generation of waste should be avoided or minimised wherever possible. Dispose of surplus and nonrecyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.
No information provided on hazardous wastes.

SECTION 14. TRANSPORT INFORMATION

General:

The product is not covered by international regulations on the transport of dangerous goods.

SECTION 15. REGULATORY INFORMATION

CHEMICAL SAFETY REPORT HAS BEEN PERFORMED FOR TEREPHTHALIC ACID. Exposure scenarios was not performed in the CSR (see Annex 2).

KEY LITERATURE REFERENCES AND SOURCES

EU DIRECTIVES

REGULATION (EC) No 1907/2006 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC.

Regulation (EC) No 1272/2008 REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Regulations. Commission regulation (EU) no 453/2010 of 20 May 2010 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH).

DIRECTIVE 1999/45/EC OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 31 May 1999 concerning the approximation of the laws, regulations and administrative provisions of the Member States relating to the classification, packaging and labelling of dangerous preparations



Directive 67/548/EEC on the approximation of the laws, regulations and administrative provisions relating to the classification, packaging and labeling of dangerous substances.
COMMISSION DECISION of 16 January 2001 amending Decision 2000/532/EC as regards the list of wastes (notified under document number (2001/118/EC).

UK REGULATORY REFERENCES

Chemicals (Hazard Information & Packaging) Regulations. The Control of Substances Hazardous to Health Regulations 1988. Health and Safety at Work Act 1974.

ENVIRONMENTAL LISTING

Control of Pollution Act 1974.

STATUTORY INSTRUMENTS

Notification of New Substances Regulations (NONS) 1993. The Export and Import of Dangerous Chemicals Regulations 2005 number 928.

APPROVED CODE OF PRACTICE

Classification and Labelling of Substances and Preparations Dangerous for Supply (EU 2001/59/EC). Safety Data Sheets for Substances and Preparations (REACH).

GUIDANCE NOTES

Workplace Exposure Limits EH40. Introduction to Local Exhaust Ventilation HS(G)37. CHIP for everyone HSG(108).

NATIONAL REGULATIONS

The Chemicals (Hazard Information and Packaging for Supply) Regulations 2002. No. 1689.
Workplace Exposure Limits 2005 (EH40).

The Carriage of Dangerous Goods and use of transportable pressure equipment regulations 2004.
Control of Substances hazardous to health regulations 2002 (as amended).

NATIONAL REGULATIONS (GERMANY)

Major Accident Hazard Legislation 82/501/EWG.

SECTION 16. OTHER INFORMATION

16.1. Indication of changes

VERSION	Date of change	Section	Description of changes
Version: 1.0	08/02/2010	All	Version was created at first
Version: 2.1	08/02/2011	All	Version created according to Regulation (EC) No 1272/2008 (Regulation CLP) & 453/2010
Version: 2.2	01/07/2013	8; 16.	Section 8, 16 were fully updated

16.2 Abbreviations and acronyms

ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
AGS	The German Committee on Hazardous Substances (Ausschuss für Gefahrstoffe – AGS)
BCF	Bioconcentration factor

DFG	Germany Research Foundation
DNEL	Derived No Effect Level
IMDG	International Maritime Dangerous Goods
ICAO-TI	Technical Instructions for the Safe Transport of Dangerous Goods by Air
K _{oc}	Adsorption coefficient
K _{ow}	octanol-water partition coefficient
LC50	Lethal Concentration to 50 % of a test population
LD50	Lethal Dose to 50% of a test population (Median Lethal Dose)
LOAEC	Lowest Observable Adverse Effect Concentration
LTEL	Long Term Exposure Limit
NIOSH	National Institute for Occupational Safety and Health (USA CDC)
NOEC	No Observed Effect Concentration
NOAEL	No Observed Adverse Effect Level
OECD	Organization for Economic Co-operation and Development
OSHA	Occupational Safety & Health Administration (USA)
PNEC	Predicted No Effect Concentration
PBT	Persistent, bioaccumulative, toxic chemical
vPvB	Very Persistent, Very Bioaccumulative
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail
STEL	Short Term Exposure Limit
STOT	Specific Target Organ Toxicity
(STOT) RE	Repeated Exposure
(STOT) SE	Single Exposure
TWA	Time Weighted Average
UN	United Nations
WGK	Wassergefährdungsklasse (<i>German: Water Hazard Class</i>)

16.3 Relevant R-phrases, Hazard- and EU Hazard-statements

None.

Safety Advice (S-phrases):

None.

Hazard statement:

None.

Precautionary statements:

None.

DISCLAIMER

This information is based on our current level of knowledge. This information may be subject to revision as new knowledge and experience becomes available, and SIBUR makes no warranties and assumes no liability in connection with any use of this information. Since SIBUR cannot be aware of all aspects of your business and the impact the REACH Regulation has for your company, SIBUR strongly encourages you to get familiar with the REACH Regulation in order to comply with its requirements and timelines.

Annex 1
Relevant identified uses of the substance

Uses by workers in industrial settings

Identified use	Process category (PROC)	Product Category (PC)	Sector of Use (SU)	Environmental Release Category (ERC)
ES1 - Industrial manufacture of polymers	PROC1, PROC2, PROC3, PROC4, PROC5, PROC7, PROC8a, PROC8b, PROC9, PROC15, PROC24	PC32	SU3 SU10	ERC1, ERC2, ERC6a, ERC6c, ERC6d
ES2 - Industrial manufacture of esters	PROC1, PROC2, PROC3, PROC4, PROC5, PROC7, PROC8a, PROC8b, PROC9, PROC15, PROC24	PC19	SU3 SU10	ERC1, ERC2, ERC6a, ERC6c, ERC6d
ES3 - Laboratory Chemicals	PROC9, PROC 10, PROC 11, PROC15	PC21	SU22	N/A
ES4 - Industrial manufacture of terephthalic acid	PROC1, PROC2, PROC3, PROC4, PROC5, PROC7, PROC8a, PROC8b, PROC9, PROC15, PROC24	PC32	SU3 SU8 SU9	ERC1, ERC2, ERC6a, ERC6c, ERC6d
ES5 - Industrial distribution of terephthalic acid	PROC1, PROC2, PROC3, PROC4, PROC5, PROC7, PROC8a, PROC8b, PROC9, PROC15, PROC24	PC32	SU3 SU8 SU9	ERC1, ERC2, ERC6a, ERC6c, ERC6d

Annex 2

Exposure assessment

Workers exposure

The need to carry out an human health exposure assessment and risk characterisation for Terephthalic acid was assessed under the terms of the ECHA document “Guidance on information requirements and chemical safety assessment” Part B, draft chapter B.8 which deals with the scope of the exposure assessment.

According to this guidance chapter, it is not required to carry out an exposure assessment and risk characterisation for human health if it can be demonstrated that there is “no hazard” for the human populations. In order to assess the need or not to conduct an exposure assessment it is important to review the human health related endpoint and to establish as to whether or not there is a potential risk to humans when using the substance. The guidance sets out some criteria in a flow chart as follows:

- 1 - Under Section 8, it was established that Terephthalic acid is not a PBT (or vPvB) substance. Therefore, it can be concluded that exposure assessment and risk characterisation should not be required.
- 2 - The substance is not classified for acute and long term toxicity (systemic and local effects) according to Directive 67/548/EEC and Regulations (EC) 1272/2008). Therefore, it can be concluded that exposure assessment and risk characterisation should not be required.
- 3 – There are no additional systemic effects that would trigger a potential risk to be controlled. In the rat, the critical effect of oral exposure is urolithiasis, the formation of urinary calculi and secondary effects on the urinary system including inflammation, hyperplasia, haematuria and increased kidney weights and was reported at dose levels above 250 mg/kg bw/day. Effects at high dose levels (1000 mg/kg bw/day) resulted in mortality. However, the relevance of these effects to humans is questionable since, for anatomical reasons, rodents are more susceptible to urolithiasis than humans. In addition, the human population will not be exposed to concentration as high as administered to the rats. Therefore, it is unlikely that the human population would be at risk when using Terephthalic acid.

Based on the above, it can be concluded that Terephthalic acid does not pose a risk to the human populations and meets the criteria for classification of “no hazard” according to REACH. No further investigation is therefore required.

Consumer exposure

As discussed above Terephthalic acid is considered to be non-hazardous to human health based on the REACH characterisation criteria. As such no exposure estimation for the consumer exposure is required.

Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties, ready biodegradation and hydrolysis in water. Therefore, the risk of secondary/indirect exposure is expected to be negligible. Terephthalic acid is readily biodegradable.

Terephthalic acid may therefore be expected to degrade rapidly, and to be completely mineralised, i.e. converted to CO₂ and H₂O without forming any recalcitrant metabolites. Terephthalic acid and its degradation intermediates are non-persistent therefore, indirect exposure of humans could not occur. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

Environmental exposure

The need to carry out an environmental exposure assessment and risk characterisation for Terephthalic acid has been assessed under the terms of the ECHA document “Guidance on information requirements and chemical safety assessment” Part B, draft chapter B.8 which deals with the scope of the exposure assessment.

This guidance chapter sets out the criteria for which a classification of “no hazard” may be derived for the purposes of REACH and relates the classification to the need to carry out the exposure assessment. It is considered that Terephthalic acid meets all the criteria thus allowing a classification of “no hazard” for the environment to be derived and, as such, it is determined that no risk characterisation for the environment is required. Details of the relevant properties of Terephthalic acid which determine the lack of any hazard are listed below. The risk of exposure of man via inhalation is dealt with separately in the human/worker exposure assessment sections.

In order to derive a classification of “no hazard” for the environment the following criteria (which are well below the classification of dangerous in accordance with directive 67/548/EEC and Regulations (EC) 1272/2008) should be met:

1. The substance should be readily biodegradable. As demonstrated in section 4.1.2.1.2 Terephthalic acid may be considered readily biodegradable based on the results of two key studies. In these studies, performed in accordance with OECD ready biodegradability guidelines, the mineralisation of Terephthalic acid comfortably exceeded the relevant pass criteria. As such, it is considered that this classification criterion is met.
2. The substance should have a very low potential for bioaccumulation with a log K_{ow} less than 2 and/or a BCF of less than 10. In public literature, Terephthalic acid has a known BCF value of 2.00 (Hansch, C. *et al.*, 1995). The potential for Terephthalic acid to bioaccumulate in the tissues of organisms that inhabit aquatic or terrestrial matrices contaminated with TPA is therefore negligible. The risk that Terephthalic acid may biomagnify through successive trophic levels of aquatic or terrestrial food chains is consequently also negligible.
3. The aquatic toxicity should fulfil both of the following conditions:
 - a. Acute EC₅₀ or LC₅₀ values should be >water solubility. TPA is slightly soluble in water (0.1 – 100 mg/L). The water solubility of TPA is 17 mg/L at 25 °C. The LC₅₀ in fish, algae and daphnia is greater than the water solubility therefore this criterion is met.

Acute toxicity studies in Daphnia derived EC₅₀ values of up to 967 mg/L which indicates no potential for toxicity.

Three reliable, GLP-compliant short-term studies are available in which TPA was treated with NaOH solution to convert the free acid to its highly soluble sodium terephthalate salt(s) prior to exposure to fish, daphnia and algae. No adverse effects occurred in these studies, up to and including the highest nominal TPA-equivalent concentrations of 1000 mg/L. The

lowest endpoint from these three studies (the 72-h E_rC_{50} for growth inhibition of *D. subspicatus*) was >668 mg TPA-equiv/L (mean measured). These studies demonstrate the low intrinsic toxicity of terephthalate to aquatic biota, and - taking into account its susceptibility to rapid biodegradation - provide assurance that Terephthalic acid does not present a long-term and/or delayed danger to the structure and/or functioning of aquatic ecosystems.

b. Chronic/long-term NOECs should be greater than 10 mg/L. A study of the chronic toxicity of Terephthalic acid on the reproduction of *Daphnia magna* provided a NOEC value of 19.5 mg/L. The 72 and 96-hour NOEC values for effects on the growth rate of two species of freshwater algae are 19 and 668 mg/L respectively. In all cases the NOEC was the highest concentration tested.

It is considered that Terephthalic acid comfortably meets the above criteria for the aquatic compartment and no toxicity risk for aquatic organism is indicated.

In addition to these criteria no risk to the terrestrial environment is indicated for Terephthalic acid based on the studies presented in section 7.2 CSR and there is no evidence for endocrine activity. As TPA is readily biodegradable the effect of the substance on soil macroorganisms is negligible.

Given the above parameters it can be concluded that Terephthalic acid poses no risk to the environment and as such as classification of “no hazard” may be derived based in the REACH criteria. In addition to this it can be concluded based on the relevant guidance document that there is no need to assess the oral exposure of man via the environment. As such no exposure assessment or risk characterisation is presented or required for risk to the environment or risk to man via the environment.



Risk characterisation

Human health

Workers

Terephthalic acid does not pose any hazard to the worker based on the strict REACH classification criteria. As such no worker exposure assessment or risk characterisation is required. As such the RCRs are not derived as no risk to the worker is indicated for Terephthalic acid.

Consumers

Terephthalic acid does not pose any hazard to the consumer based on the strict REACH classification criteria. As such no consumer exposure assessment or risk characterisation is required. As such the RCRs are not derived as no risk to the consumer is indicated for Terephthalic acid.

Indirect exposure of humans via the environment

Terephthalic acid does not pose any hazard humans via the environment based on the strict REACH classification criteria. As such no exposure assessment or risk characterisation is required for humans via the environment.

Environment

Terephthalic acid does not pose any hazard to the environment based on the strict REACH classification criteria. As such no environmental exposure assessment or risk characterisation is required. As such environmental RCRs are not derived as no risk to the environment is indicated for Terephthalic acid.

END OF SDS