

# Safety data sheet according to 1907/2006/EC, Article 31

Printing date: 21.05.2017

Version: 1.0

Revision: 21.05.2017

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

- 1.1 Product identifier
- Trade name: <u>4-tert-butylbenzoic acid (PTBBA)</u>
- · CAS Number:
- 98-73-7
- EC number: 202-696-3 Reach Registration Number (Intermediate): 01-2120762776-40-0000 TII <1000 MT
- · 1.2 Application of the substance / the preparation:
- Cosmetics Intermediates, Catalyst for alkyd resins, PVC Stabiliser, Additives to Lubricants, Flavors & Fragrance, Antioxidants etc.
- $\cdot$  1.3 Details of the supplier of the safety data sheet
- · Details of the supplier of the safety data sheet
- Manufacturer/Supplier:
  Vinati Organics Limited,
  Regd Add: B-12 & B-13/1, MIDC, Mahad-402309
  Parinee Crescenzo, 11th floor, 'G' block,
  Behind MCA, Bandra Kurla Complex,
  Bandra (E), Mumbai 400051,India Ph: +91 22 61240422
  Further information obtainable from: 09765667972

## **SECTION 2: Hazards identification**

#### · Classification according to Regulation (EC) No 1272/2008

Dermal.

GHS08 health hazard

Repr. 1B H360F May damage fertility.

STOT RE 1 H372 Causes damage to the central nervous system, the kidneys, the liver, the thymus, the testes and the hemopoietic system through prolonged or repeated exposure. Route of exposure: Oral, Inhalative,



Aquatic Chronic 2 H411 Toxic to aquatic life with long lasting effects.



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- · 2.3 Other hazards Aqueous solutions of the substance are acidic.
- · Results of PBT and vPvB assessment
- · PBT: Substance characteristics do not meet screening criteria.
- · vPvB: Substance characteristics do not meet screening criteria.

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# **SECTION 3: Composition/information on ingredients**

- · 3.1 Chemical characterization: Substances
- CAS No. Description:
- 98-73-7 4-tert-butylbenzoic acid
- · Identification number(s):
- · EC number: 202-696-3

## **SECTION 4: First aid measures**

## · 4.1 Description of first aid measures

#### · General information:

Symptoms of poisoning may occur even after several hours; therefore medical observation is suggested for at least 48 hours after the accident.

Immediately remove any clothing soiled by the product.

#### After inhalation:

Remove victim from contaminated area. If breathing is difficult, give oxygen. If breathing stops, provide artificial respiration. Call a doctor.

In case of unconsciousness, place patients on their side in a stable position for transportation.

After skin contact:

Clean affected skin thoroughly with water and a mild cleansing agent. No residues shall remain on the skin.

If available, apply polyethylenglycol (PEG 400, Lutrol) and let it remain on the skin for several minutes.

Do not use solvents or thinners.

Seek medical treatment.

- After eye contact: Rinse the eyes with open eyelids for 10 15 minutes with water. Then consult a doctor (eye specialist).
- · After swallowing:
- Rinse mouth with water.
- Spit liquid out again.

Never give anything by mouth to an unconscious person.

Do not induce vomiting.

If vomitting occurs spontaneously:

A person vomiting while lying on the back should be turned onto the side.

Hold the head of the vomiting person low with the body in a prone position in order to avoid aspiration.

Call a doctor immediately.

#### · 4.2 Most important symptoms and effects, both acute and delayed

After inhalation: Cough Dyspnoea

After swallowing: After resorption:

Ataxia

4.3 Indication of any immediate medical attention and special treatment needed

Symptomatic treatment

(decontamination, vital functions)

In cases of irritation to the lungs, initial treatment with Dexametason metered aerosol

# **SECTION 5:** Firefighting measures

· 5.1 Extinguishing media

#### · Suitable extinguishing agents:

CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

- Use fire fighting measures that suit the environment.
- · For safety reasons unsuitable extinguishing agents: High volume water jet
- · 5.2 Special hazards arising from the substance or mixture

In case of fire, the following can be released:



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Carbon monoxide (CO) Carbon dioxide (CO<sub>2</sub>) Irritant gases/vapours

· 5.3 Advice for firefighters

· Protective equipment: Wear self-contained respiratory protective device.

· Additional information:

Heating leads to pressure increase entailing danger of bursting and explosion. Immediately cool neighbouring packages and containers with sprayed water and, if possible, remove them out of the danger zone

Dispose of fire debris and contaminated fire fighting water in accordance with official regulations.

Collect contaminated fire fighting water separately. It must not enter the sewage system.

#### **SECTION 6: Accidental release measures**

#### · 6.1 Personal precautions, protective equipment and emergency procedures



Wear protective equipment. Keep unprotected persons away.

#### Ensure adequate ventilation.

Avoid formation of dust.

Use respiratory protective device against the effects of fumes/dust/aerosol.

Do not smoke - keep ignition sources away

#### 6.2 Environmental precautions:

Do not allow product to reach sewage system or any water course.

Inform respective authorities in case of seepage into water course or sewage system.

Do not allow to penetrate the ground/soil.

# In case of seepage into the ground inform responsible authorities.

 $\cdot$  6.3 Methods and material for containment and cleaning up:

Ensure adequate ventilation.

Avoid any dust formation. Pick up with a tested and approved industrial vacuum cleaner if necessary.

Make sure to recycle or dispose of in suitable receptacles.

#### 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

It is recommended to handle and refill product in closed systems.

If this is not possible:

Ensure good ventilation/exhaustion at the workplace.

Prevent formation of dust.

Any deposit of dust which cannot be avoided must be regularly removed.

Avoid inhalation of dust.

Avoid contact with eyes and skin.

Restrict the quantity stored at the work place.

Observe the special requirements for handling carcenogenic, mutagenic chemical substances and those toxic to reproduction as outlined in directive 90/394/EEC in its current version.

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### · Information about protection against explosions and fires:

Keep ignition sources away - Do not smoke.

Protect against electrostatic charges.

- · 7.2 Conditions for safe storage, including any incompatibilities
- · Storage:
- Requirements to be met by storerooms and receptacles:

Store container tightly sealed at a cool and dry place with sufficient ventilation.

- Prevent any seepage into the ground.
- · Information about storage in one common storage facility: Store away from foodstuffs.
- Store away from feed.
- Refer to national regulations for storing hazardous chemicals.
- · Further information about storage conditions:
- Keep receptacle tightly sealed.
- Store under lock and key and with access restricted to technical experts or their assistants only.
- Storage class: 6.1C: Combustible substances, acute toxic cat. 3/toxic or having chronic effects
- · 7.3 Specific end use(s) No further relevant information available

### **SECTION 8: Exposure controls/personal protection**

- · Additional information about design of technical systems: No further data; see section 7.
- 8.1 Control parameters
- · Components with limit values that require monitoring at the workplace: Not required
- · DNELs Abbreviations: In = Industrial Prof = Professional Cons = Consumer

LLE = Long term, local effects LSE = Long term, systemic effects SLE = Short term, local effects SSE = Short term, systemic effects Oral DNEL/Cons/LSE 1.6 mg/kg bw/day (human) Inhalative DNEL/In/LSE 0.067 mg/m3 (human) DNEL/In/SSE 1.2 mg/m<sup>3</sup> (human)

## · DMELs

Abbreviations: In = Industrial Prof = Professional Cons = Consumer

LLE = Long term, local effects LSE = Long term, systemic effects SLE = Short term, local effects SSE = Short term, systemic effects Dermal DMEL/Cons/LSE 7.5 mg/kg bw/day (human) DMEL/In/LSE 0.017 mg/kg bw/day (human) DMEL/In/SSE 0.15 mg/kg bw/day (human)

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(Contd. of page 5) · PNECs Since the substance has no potential for bioaccumulation no PNEC oral was derived. Abbreviations: aq = aqua sed = sediment PNEC 7.36 µg/l (soil) PNEC STP 32 mg/L (sewage treatment plant) PNEC/Aq 24 µg/l (fresh water) 240 mg/l (intermittent release) 2.4 µg/l (marine water) PNEC/sed 30.1 µg/kg (fresh water) 3.01 µg/kg (marine water) · Additional information: The lists that were valid during the creation were used as basis. 8.2 Exposure controls · Personal protective equipment: General protective and hygienic measures: Keep away from foodstuffs, beverages and feed. Do not eat or drink while working. Avoid contact with eyes and skin. Wash hands before breaks and at the end of work. Vacuum contaminated clothing. Do not blow or brush off contamination. Remove all soiled and contaminated clothing immediately. Do not inhale dust/smoke/mist. After skin contact, cleanse skin thoroughly. Ensure that washing facilities are available at the work place. After contact with eyes, rinse immediately. Provide eye bath. **Breathing equipment:** In case of unintentional release of substance, exceeding the occupational exposure limit value: In case of brief exposure or low pollution use a respiratory filter device. In case of intensive or longer exposure use a respiratory protective device that is independent of circulating air. Short term filter device (EN 149): Filter P3 Breathing equipment is only to be used in order to handle the residual risk of short term jobs if all other risk minimizing measures have been carried out e.g. retention and/or local exhaust. Protection of hands: Chemical resistant gloves (EN 374) The glove material has to be impermeable and resistant to the product/substance/preparation. Selection of the glove material in consideration of the penetration times, rates of diffusion and the degradation After use of gloves apply skin-cleaning agents and skin cosmetics. 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: > 480 min The above-mentioned times are based on reference values as per EN 374. Under practical conditions (33 °C - taking into account the body temperature), the maximum wearing time is to be limited to one-third. · For the permanent contact gloves made of the following materials are suitable:

For example protection gloves made by KCL GmbH, D-36124 Eichenzell; email: vertrieb@kcl.de, with following specification (tested according to EN 374): Material: natural rubber

Thickness: 0.5 mm Permeation time: > 480 min

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Product name: Cama Clean (708) Material: Nitrile Thickness: 0.4 mm Permeation time: > 480 min Product name: Camatril-Velours (730) Material: special nitrile Thickness: 0.16 mm Permeation time: 480 Min Product name: SivoChem 759 (759) Material: Nitrile, nitrile foam, cotton Thickness: 1.65 mm Permeation time: 480 Min Product name: TevuChem 763 (763) These recommendations are valid only for the product mentioned in this safety data sheet. · As protection from splashes gloves made of the following materials are suitable: For example protection gloves made by KCL GmbH, D-36124 Eichenzell; email: vertrieb@kcl.de, with following specification (tested according to EN 374): Material: natural rubber Thickness: 1 mm Permeation time: > 480 Min Product name: Combi-Latex (395) Material: polychloroprene with natural rubber Thickness: 0.6 mm permeation time: > 60 min Product name: Camapren (720) These recommendations are valid only for the product mentioned in this safety data sheet. · Eye protection: Goggles recommended during refilling · Body protection: Protective work clothing According to hazard: Apron

Boots

# **SECTION 9: Physical and chemical properties**

• 9.1 Information on basic physical and c	hemical properties	
· Appearance:		
Form:	Crystalline	
Colour:	White	
· Odour:	Aromatic	
· Odour threshold:	Not determined	
· pH-value (0.07 g/l) at 20 °C:	~ 3.9	
· Change in condition:		
Melting point/Melting range:	165-167 °C	
Boiling point/Boiling range:	280 °C	
	Decomposition	
· Flash point:	Not applicable	
· Flammability (solid, gaseous):	Product is not flammable.	
· Ignition temperature:		
Decomposition temperature:	> 280 °C	
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· Danger of explosion:	Product is not explosive. However, formation of explosive air/dust mixtures is possible.	
· Explosion limits:		
Lower:	Not applicable	
Upper:	Not applicable	
<ul> <li>Oxidizing properties:</li> </ul>	None	
<ul> <li>Vapour pressure at 20 °C:</li> </ul>	0.057 hPa	
· Density at 20 °C:	1.142 g/cm <sup>3</sup>	
<ul> <li>Dissociation constant pKa at 25 °C</li> </ul>	4.36	
· Solubility in / Miscibility with		
Water at 20 °C:	12.6 g/l	
· Partition coefficient (n-octanol/water) at 21 °C: 3.4 log POW		
	Experimental	
· Viscosity:		
dynamic:	Not applicable	
kinematic:	Not applicable	
Surface tension:	Not relevant	
· 9.2 Other information	No further relevant information available	

## **SECTION 10: Stability and reactivity**

- · 10.1 Reactivity No further relevant information available
- · 10.2 Chemical stability
- · Thermal decomposition / conditions to be avoided:
- No decomposition if used and stored according to specifications
- To avoid thermal decomposition do not overheat.
- · 10.3 Possibility of hazardous reactions Violent reactions possible with below mentioned substances
- · 10.4 Conditions to avoid No further relevant information available
- · 10.5 Incompatible materials:

Strong oxidants

Strong bases

· 10.6 Hazardous decomposition products:

No hazardous decomposition products if instructions for storage and handling are followed

# **SECTION 11: Toxicological information**

#### 11.1 Information on toxicological effects

· Acute toxicity:

LD/LC50 values that are relevant for classification: LD<sub>50</sub> 568 mg/kg (mouse) Oral intragastical administration ~ 300 mg/kg (rat) Dermal  $LD_{50}$ LD50 (rabbit): > 2000 mg/kg According to EU risk assessment report of 2009 (TC C&L in September 2007) the available LD50 for dermal application was not sufficient for classification. Inhalative LC<sub>50</sub>/4 h > 1.802 mg/l (rat) Exposition to dust of PTBBA According to EU risk assessment report of 2009 (TC C&L in September 2007) the available LC50 for inhalation was not sufficient for classification. (Contd. on page 9)



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<ul> <li>Primary</li> <li>on the sl No irritati (84/449/E</li> <li>on the ey No irritati (84/449/E</li> <li>On respi</li> <li>Sensitiza</li> <li>Other inf</li> <li>Carcinog Carcinog No classi Ames-tes Mutageni</li> </ul>	irritant effect: kin: ng effect EWG appendix V ye: ng effect EWG appendix V ratory tract: No ation: No sensiti formation (abou genic, mutageni enicity: fication st: negative icity (mammaliar	<sup>7</sup> B4) <sup>7</sup> B5) data available zation species: guinea pig OECD 406 at experimental toxicology): ic effects and adverse effects on reproduction:	
Mutageni	city (mammaliar	cell test): chromosomes aberration negative (OECD 475)	
Mutageni	city:		
Toxicity t	o reproduction.		
Oral	NOAEL	1.6 mg/kg bw/day (rat) Toxicity to reproduction	
Dermal	NOAEL	30 mg/kg bw/day (rat) Toxicity to reproduction	
Inhalative	e LOAEC (mater	nal) 12.5 mg/m³ (rat) Toxicity to reproduction	
<ul> <li>Subacutt</li> <li>STOT-sin</li> <li>STOT-re Route of Oral</li> <li>Dermal</li> <li>Inhalative</li> <li>Effected</li> <li>Central n</li> <li>Liver</li> <li>Kidneys</li> <li>Testes</li> <li>Epididym</li> <li>Hemopoi</li> <li>Thymus</li> <li>Aspiration</li> <li>Repeated</li> <li>Oral</li> </ul>	e to chronic tox ngle exposure in peated exposure exposure: ervous system ides etic system on hazard No cla al toxicological dose toxicity: LOAEL 6 mg/kg	Assification e: assification information: Risk of skin absorption g bw/d (rat) opic study (90 days)	
Dormal	subchr	onic study (90 days)	
Dermal	subchr	onic, extrapolation to 90 days	
Inhalative	Inhalative LOAEC 1.5 mg/m³ (rat) subchronic, extrapolation to 90 days		
· CMR effe Repr. 1B	ects (carcinoge	nity, mutagenicity and toxicity for reproduction):	

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# **SECTION 12: Ecological information**

#### · 12.1 Toxicity

#### · Aquatic toxicity:

- EC<sub>50</sub> > 1000 mg/l (activated sludge, domestic) (88/302/EEC, Part C11 and OECD 209)
- EC<sub>50</sub>/24h (static) 47 mg/l (Daphnia magna)
- EC<sub>50</sub>/48h (static) 24 mg/l (Daphnia magna)

EC<sub>50</sub>/72h > 94 mg/l (Pseudokirchneriella subcapitata) (OECD 201; 92/69/EC, C3)

LC<sub>50</sub>/96h 33 mg/l (Carrassius auratus)

pH value 7; LC50 (96h, pH 5): 4 mg/L

320 mg/l (Oncorhynchus mykiss)

semi-static

· 12.2 Persistence and degradability No further relevant information available

#### · Other information:

Not readily biodegradable

- OECD 301 D
- · 12.3 Bioaccumulative potential Due to the distribution coefficient n-octanol/water an accumulation in organisms is not expected.
- · 12.4 Mobility in soil No further relevant information available
- · Ecotoxical effects:
- · Remark: Toxic to fish
- · Additional ecological information:
- · General notes:

Water danger class 3 (German Regulation) (Self-assessment): extremely hazardous to water

- Do not allow product to reach ground water, water course or sewage system, even in small quantities.
- Danger to drinking water even if extremely small quantities leak into the ground.
- Also poisonous for fish and plankton in water bodies
- Toxic to aquatic organisms
- · 12.5 Results of PBT and vPvB assessment
- $\cdot$  PBT: Substance characteristics do not meet screening criteria.
- · vPvB: Substance characteristics do not meet screening criteria.
- · 12.6 Other adverse effects No further relevant information available

#### **SECTION 13: Disposal considerations**

#### · 13.1 Waste treatment methods

#### · Recommendation:

Must not be disposed of together with household garbage. Do not allow product to reach sewage system. Must be recycled or disposed of according to the regulations. Waste has to be classified according to the European Waste Catalogue based on the identification of the waste generating source.

#### European waste catalogue:

07 00 00 WASTES FROM ORGANIC CHEMICAL PROCESSES

07 01 00 wastes from the manufacture, formulation, supply and use (MFSU) of basic organic chemicals

07 01 04\* other organic solvents, washing liquids and mother liquors

#### · Uncleaned packagings:

#### Recommendation:

Disposal must be made according to official regulations.

Packagings that cannot be cleaned are to be disposed of in the same manner as the product.

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SECTION 14: Transport information	
· 14.1 UN-Number · ADR, IMDG, IATA	UN3077
<ul> <li>14.2 UN proper shipping name</li> <li>ADR</li> </ul>	3077 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4-
· IMDG	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4-tert- butylbenzoic acid), MARINE POLLUTANT
	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4-tert- butylbenzoic acid)
14.3 Transport hazard class(es)	
ADR	
· Class · Label	9 (M7) Miscellaneous dangerous substances and articles. 9
· IMDG, IATA	
· Class · Label	9 Miscellaneous dangerous substances and articles. 9
<ul> <li>14.4 Packing group</li> <li>ADR, IATA</li> </ul>	ш
14.5 Environmental hazards: Marino pollutant:	Symbol (fish and trac)
· Special marking (ADR):	Symbol (fish and tree)
· Special marking (IATA):	Symbol (fish and tree)
14.6 Special precautions for user     Danger code (Kemler):     EMS Number:	Warning: Miscellaneous dangerous substances and articles. 90
• 14.7 Transport in bulk according to Annex II o	f
MARPOL73/78 and the IBC Code	Not applicable
· Transport/Additional information:	
· ADR	5 kg
· Transport category:	3
• Tunnel restriction code:	E
· IATA · Remarks:	Packing Instructions: For Limited Quantities: Y956 (Max Net Qty/Pkg: 30 kg G) Passenger and Cargo Aircraft: 956 400 kg Cargo Aircraft only: 956 400 kg
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· UN "Model Regulation":

UN3077. ENVIRONMENTALLY HAZARDOUS SUBSTANCE. SOLID. N.O.S. (4-tert-butylbenzoic acid), 9, III

### **SECTION 15: Regulatory information**

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

#### National regulations

· Information about limitation of use:

The number of employees handling this chemical substance has to be kept as small as possible.

Take note of Directive 92/85/EC on the safety and health of pregnant workers at work.

Take note of Directive 94/33/EC on the protection of young people at work.

#### · Water hazard class:

Ident number.: 5573

Water danger class 3 (Self-assessment): extremely hazardous for water

- Other regulations, limitations and prohibitive regulations: REACH regulation (EC) 552/2009 Annex XVII
- · 15.2 Chemical safety assessment: A chemical Safety Assessment has been carried out.

#### **SECTION 16: Other information**

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

#### Abbreviations and acronyms:

ICAO: International Civil Aviation Organization

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of

Dangerous Goods by Rail)

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

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

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 \* Sources: Toxnet ChemID
 ESIS (EU Existing Substances Information System) Chemical Safety Report (Contd. of page 12)

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## Annex: Exposure scenario 1

· Short title of the exposure scenario Distribution of the substance (industrial) · Sector of Use SU3 Industrial uses: Uses of substances as such or in preparations at industrial sites · Process category PROC1 Use in closed process, no likelihood of exposure PROC2 Use in closed, continuous process with occasional controlled exposure PROC3 Use in closed batch process (synthesis or formulation) PROC8b Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC15 Use as laboratory reagent · Environmental release category ERC2 Formulation of preparations · Conditions of use · Worker ≤ 8 h/d (PROC 1, 2, 3, 8b, 15) · Physical parameters · Physical state Solid Powder dustiness: high Remark to physical state: "dustiness: high" and "dustiness: low" are assumptions for the calculation of the exposition, whereas "dustiness: high" is a conservative assumption - a higher degree of dustiness increases the hazard of exposition. Used amount per time or activity ≤ 25 tonnes per day and site ≤ 500 tonnes per year and site Other operational conditions Other operational conditions affecting environmental exposure Receiving surface water flow rate: ≥ 18000 m3/d Municipal sewage treatment plant (STP) Discharge rate of sewage treatment plant (STP): ≥ 2000 m3/d application of the STP sludge on agricultural soil Other operational conditions affecting worker exposure place of use: indoors: PROC 1, 2, 8b, 15 assumption of exposed body surface: palm of one hand: 240 cm2 (PROC 1, 3, 15) Assumed exposed body surface: palm of both hands: 480 cm2 (PROC 2, 8b) Local exhaust ventilation: PROC 2, 3, 8b, 15 Effectiveness local exhaust ventilation: 90 % (PROC 2, 3, 8b, 15) Local exhaust ventilation, close to emission source: PROC 8b Effectiveness of local exhaust ventilation close to emission source: 80 % (PROC 8b) Effectiveness, use of closed containers and systems: 80 % (PROC 3) Respiratory protection: PROC 2, 8b, 15 Effectiveness of respiratory protection (a): 90 % (PROC 2, 15) Effectiveness of respiratory protection (b): 95 % (PROC 8b) Protective gloves: PROC 1, 2, 8b, 15 Effectiveness of protective gloves: 95 % (PROC 2, 8b, 15) Effectiveness of protective gloves: 98 % (PROC 1) · Risk management measures · Worker protection Organisational protective measures Exposure must be kept under the limits of the highest expected concentrations (see under "Exposure estimation") · Environmental protection measures Exposure must be kept under the limits of the highest expected concentrations (see under "Exposure estimation") Exposure estimation · Worker (dermal) The highest expected concentration of dermal exposition is 0.007 mg/kg bw/d. (a) PROC 1, 2, 3, 8b; RCR=0.403)



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(Contd. of page 14) The highest expected concentration of dermal exposition is 0.002 mg/kg bw/d. (b) PROC 15; RCR=0.101) · Worker (inhalation) The highest expected concentration of inhalative exposition is 0.01 mg/m3. (a) PROC 1, 2; RCR=0.149) The highest expected concentration of inhalative exposition is 0.02 mg/m3. (b) PROC 3; RCR=0.298) The highest expected concentration of inhalative exposition is 0.012 mg/m3. (c) PROC 8b; RCR=0.185) The highest expected concentration of inhalative exposition is 0.05 mg/m3. (d) PROC 15; RCR=0.746) Environment Estimated/calculated release into the environment (freshwater) after risk management measures: 0.09 kg/d Estimated/calculated release into the environment (air) after risk management measures: 0.05 kg/d Estimated/calculated release into the environment (soil) after risk management measures: 0.01 % The highest expected concentration for the environmental exposition (local PEC) of freshwater is 0.00672 mg/L. (ERC 2; RCR=0.28) The highest expected concentration for the environmental exposition (local PEC) of freshwater sediment is 0.0282037 mg/kg dry weight. (ERC 2; RCR=0.937) The highest expected concentration for the environmental exposition (local PEC) of marine water is 0.0006696 mg/L. (ERC 2; RCR=0.279) The highest expected concentration for the environmental exposition (local PEC) of marine water sediment is 0.00281134 mg/kg dry weight. (ERC 2; RCR=0.934) The highest expected concentration for the environmental exposition (local PEC) of STP effluent is 0.032 mg/L. (ERC 2; RCR=0.001) The highest expected concentration for the environmental exposition (local PEC) of agricultural soil is 0.00087584 mg/kg dry weight. (ERC 2; RCR=0.119) · Guidance for downstream users Risk assessment tool(s) utilised: EUSES version 2.1 ECETOC TRA workers version 2 (Contd. on page 16)



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# Trade name: 4-tert-butylbenzoic acid (PTBBA)

# Annex: Exposure scenario 2

· Short title of the exposure scenario Use as intermediate in case: Industrial manufacture of resins · Sector of Use SU3 Industrial uses: Uses of substances as such or in preparations at industrial sites · Product category PC19 Intermediate PC32 Polymer preparations and compounds · Process category PROC1 Use in closed process, no likelihood of exposure PROC2 Use in closed, continuous process with occasional controlled exposure PROC3 Use in closed batch process (synthesis or formulation) **PROC6** Calendering operations PROC8b Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC9 Transfer of substance or preparation into small containers (dedicated filling line, including weighing) PROC14 Production of preparations or articles by tabletting, compression, extrusion, pelletisation PROC15 Use as laboratory reagent · Environmental release category ERC6a Industrial use resulting in manufacture of another substance (use of intermediates) · Conditions of use · Worker ≤ 8 h/d (PROC 1, 2, 3, 6, 8b, 9, 14, 15) · Physical parameters · Physical state Solid Powder dustiness: high PROC 1, 2, 3, 8b, 15 Dustiness: moderate PROC 6 Dustiness: low PROC 9, 14 Remark to physical state: "dustiness: high" and "dustiness: low" are assumptions for the calculation of the exposition, whereas "dustiness: high" is a conservative assumption - a higher degree of dustiness increases the hazard of exposition. Used amount per time or activity ≤ 25 tonnes per day and site ≤ 500 tonnes per year and site Other operational conditions Other operational conditions affecting environmental exposure Receiving surface water flow rate: ≥ 18000 m3/d Municipal sewage treatment plant (STP) Discharge rate of sewage treatment plant (STP): ≥ 2000 m3/d application of the STP sludge on agricultural soil Other operational conditions affecting worker exposure place of use: indoors: PROC 1, 2, 3, 6, 8b, 9, 14, 15 assumption of exposed body surface: palm of one hand: 240 cm2 (PROC 1, 3, 15) Assumed exposed body surface: palm of both hands: 480 cm2 (PROC 2, 8b, 9, 14) Assumed exposed body surface: both hands: 960 cm2 (PROC 6) . . . . . . . . . . . . Use of closed containers and systems: PROC 3 Effectiveness, use of closed containers and systems: 80 % (PROC 3) Local exhaust ventilation: PROC 2, 3, 6, 8b, 9, 14, 15 Effectiveness local exhaust ventilation: 90 % (PROC 2, 3, 6, 8b, 9, 14, 15) Local exhaust ventilation, close to emission source: PROC 8b, 9 Effectiveness of local exhaust ventilation close to emission source: 80 % (PROC 8b, 9)



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# Trade name: 4-tert-butylbenzoic acid (PTBBA)

(Contd. of page 16) Respiratory protection: PROC 2, 6, 8b, 15 Effectiveness of respiratory protection (a): 90 % (PROC 2, 15) Effectiveness of respiratory protection (b): 95 % (PROC 6, 8b) . . . . . . . . . . . Protective gloves: PROC 1, 2, 6, 8b, 9, 14, 15 Effectiveness of protective gloves: 95 % (PROC 2, 6, 8b, 9, 14, 15) Effectiveness of protective gloves: 98 % (PROC 1) Protective clothing: PROC 6, 14 · Risk management measures Worker protection Organisational protective measures Exposure must be kept under the limits of the highest expected concentrations (see under "Exposure estimation") · Environmental protection measures Exposure must be kept under the limits of the highest expected concentrations (see under "Exposure estimation") · Exposure estimation · Worker (dermal) The highest expected concentration of dermal exposition is 0.002 mg/kg bw/d. (a) PROC 14, 15; RCR 0.101) The highest expected concentration of dermal exposition is 0.007 mg/kg bw/d. (b) PROC 1, 2, 3, 6, 8b, 9; RCR 0.403) Worker (inhalation) The highest expected concentration of inhalative exposition is 0.01 mg/m3. (PROC 1, 2, 14; RCR 0.149) The highest expected concentration of inhalative exposition is 0.05 mg/m3. (PROC 15; RCR 0.746) The highest expected concentration of inhalative exposition is 0.012 mg/m3. (PROC 8b; RCR 0.185) The highest expected concentration of inhalative exposition is 0.02 mg/m3. (PROC 3: RCR 0.298) The highest expected concentration of inhalative exposition is 0.025 mg/m3. (PROC 6; RCR 0.373) The highest expected concentration of inhalative exposure is 0.002 mg/m3. (PROC 9; RCR 0.030) Environment Estimated/calculated release into the environment (freshwater) after risk management measures: 0.09 kg/d Estimated/calculated release into the environment (air) after risk management measures: 0.05 kg/d Estimated/calculated release into the environment (soil) without risk management measures: 0.1 % The highest expected concentration for the environmental exposition (local PEC) of freshwater is 0.007 mg/L. (ERC 6a; RCR 0.280) The highest expected concentration for the environmental exposition (local PEC) of freshwater sediment is 0.028 mg/kg dry weight. (ERC 6a; RCR 0.937) The highest expected concentration for the environmental exposition (local PEC) of marine water is 0.000669 mg/L. (ERC 6a; RCR 0.279) The highest expected concentration for the environmental exposition (local PEC) of marine water sediment is 0.003 mg/kg dry weight. (ERC 6a; RCR 0.934) The highest expected concentration for the environmental exposition (local PEC) of STP effluent is 0.045 mg/L. (ERC 6a; RCR 0.001) The highest expected concentration for the environmental exposition (local PEC) of agricultural soil is 0.000873 mg/kg dry weight. (ERC 6a; RCR 0.119) Guidance for downstream users Risk assessment tool(s) utilised: EUSES version 2.1 ECETOC TRA workers version 2

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# Trade name: 4-tert-butylbenzoic acid (PTBBA)

## Annex: Exposure scenario 3

· Short title of the exposure scenario

Use of resins (containing PTBBA) as binding agent in manufacture of paints/coatings (industrial)

· Sector of Use SU3 Industrial uses: Uses of substances as such or in preparations at industrial sites

· Product category PC9a Coatings and paints, thinners, paint removers

· Process category

PROC1 Use in closed process, no likelihood of exposure

PROC2 Use in closed, continuous process with occasional controlled exposure

PROC3 Use in closed batch process (synthesis or formulation)

PROC8b Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC9 Transfer of substance or preparation into small containers (dedicated filling line, including weighing) PROC15 Use as laboratory reagent

- · Environmental release category ERC5 Industrial use resulting in inclusion into or onto a matrix
- · Conditions of use
- Worker ≤ 8 h/d (PROC 1, 2, 3, 8b, 9, 15)
- · Physical parameters
- Physical state
- Solid
- Powder
- dustiness: high
- PROC 1, 2, 3, 8b, 15
- Dustiness: low
- PROC 9

Remark to physical state: "dustiness: high" and "dustiness: low" are assumptions for the calculation of the exposition, whereas "dustiness: high" is a conservative assumption - a higher degree of dustiness increases the hazard of exposition.

- · Used amount per time or activity
- ≤ 25 tonnes per day and site
- ≤ 500 tonnes per year and site
- Other operational conditions
- · Other operational conditions affecting environmental exposure

Receiving surface water flow rate: ≥ 18000 m3/d

Municipal sewage treatment plant (STP) Discharge rate of sewage treatment plant (STP): ≥ 2000 m3/d

application of the STP sludge on agricultural soil

- Other operational conditions affecting worker exposure
- place of use: indoors: PROC 1, 2, 3, 8b, 9, 15

assumption of exposed body surface: palm of one hand: 240 cm2 (PROC 1, 3, 15)

Assumed exposed body surface: palm of both hands: 480 cm2 (PROC 2, 8b, 9)

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Use of closed containers and systems: PROC 3

Effectiveness, use of closed containers and systems: 80 % (PROC 3)

Effectiveness of protective gloves: 98 % (PROC 1)



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# Trade name: 4-tert-butylbenzoic acid (PTBBA)

- · Risk management measures
- Worker protection
- · Organisational protective measures

Exposure must be kept under the limits of the highest expected concentrations (see under "Exposure estimation") · Environmental protection measures

- Exposure must be kept under the limits of the highest expected concentrations (see under "Exposure estimation")
- · Exposure estimation
- Worker (dermal)

The highest expected concentration of dermal exposition is 0.002 mg/kg bw/d. (a) PROC 15; RCR 0.101)

The highest expected concentration of dermal exposition is 0.007 mg/kg bw/d. (b) PROC 1, 2, 3, 8b, 9; RCR 0.403) Worker (inhalation)

The highest expected concentration of inhalative exposition is 0.01 mg/m3. (PROC 1, 2; RCR 0.149)

The highest expected concentration of inhalative exposition is 0.05 mg/m3. (PROC 15; RCR 0.746)

The highest expected concentration of inhalative exposition is 0.012 mg/m3. (PROC 8b; RCR 0.185)

The highest expected concentration of inhalative exposition is 0.02 mg/m3. (PROC 3; RCR 0.298)

The highest expected concentration of inhalative exposition is 0.002 mg/m3. (PROC 9; RCR 0.030)

#### Environment

Estimated/calculated release into the environment (freshwater) after risk management measures: 0.09 kg/d

Estimated/calculated release into the environment (air) after risk management measures: 0.05 kg/d

Estimated/calculated release into the environment (soil) without risk management measures: 1 %

The highest expected concentration for the environmental exposition (local PEC) of freshwater is 0.007 mg/L. (ERC 5; RCR 0.280) The highest expected concentration for the environmental exposition (local PEC) of freshwater sediment is 0.028 mg/kg dry weight. (ERC 5: RCR 0.937)

The highest expected concentration for the environmental exposition (local PEC) of marine water is 0.000669 mg/L. (ERC 5; RCR 0.279)

The highest expected concentration for the environmental exposition (local PEC) of marine water sediment is 0.003 mg/kg dry weight. (ERC 5; RCR 0.934)

The highest expected concentration for the environmental exposition (local PEC) of STP effluent is 0.045 mg/L. (ERC 5; RCR 0.001)

The highest expected concentration for the environmental exposition (local PEC) of agricultural soil is 0.000873 mg/kg dry weight. (ERC 5; RCR 0.119)

#### Guidance for downstream users

Risk assessment tool(s) utilised:

EUSES version 2.1

ECETOC TRA workers version 2

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# Trade name: 4-tert-butylbenzoic acid (PTBBA)

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# Annex: Exposure scenario 4

- · Short title of the exposure scenario Use of paints / coatings with resin as binding agent containing PTBBA (professional use)
- Sector of Use SU22 Professional uses: Public domain (administration, education, entertainment, services, craftsmen)
- · Product category PC9a Coatings and paints, thinners, paint removers
- Process category PROC21 Low energy manipulation of substances bound in materials and/or articles
- · Environmental release category
- ERC10a Wide dispersive outdoor use of long-life articles and materials with low release
- ERC11a Wide dispersive indoor use of long-life articles and materials with low release
- · Conditions of use
- · Worker  $\leq$  8 h/d (PROC 21)
- Physical parameters Application temperature = Ambient temperature (PROC 21)
- · Physical state
- Solid
- Powder
- Dustiness: low
- PROC 21

Remark to physical state: "dustiness: high" and "dustiness: low" are assumptions for the calculation of the exposition, whereas "dustiness: high" is a conservative assumption - a higher degree of dustiness increases the hazard of exposition.

- · Concentration of the substance in the mixture Concentration: ≤ 0.1 % (PROC 21)
- · Used amount per time or activity
- 1 tonnes per day and site
- ≤ 500 tonnes per year and site

Remark: The given amounts refer to a single ERC respectively.

- · Other operational conditions
- · Other operational conditions affecting environmental exposure
- Receiving surface water flow rate: ≥ 18000 m3/d
- Municipal sewage treatment plant (STP)

Discharge rate of sewage treatment plant (STP): ≥ 2000 m3/d

- application of the STP sludge on agricultural soil
- Remark: The given amounts in m3/d refer to a single ERC respectively.
- · Other operational conditions affecting worker exposure
- place of use: indoors: PROC 21
- assumed exposed body surface: both hands and main part of arms: 1980 cm2 (PROC 21)
- Risk management measures
- · Worker protection
- · Organisational protective measures
- Exposure must be kept under the limits of the highest expected concentrations (see under "Exposure estimation")
- · Technical protective measures
- Ensure good ventilation/exhaustion at the workplace.
- ventilation rate (air exchange rate): 5-10 / h (PROC 21)
- · Personal protective measures
- protective/chemical resistant gloves, in combination with basic use instructions/training (PROC 21)
- effectiveness protective/chemical resistant gloves: 90 % (PROC 21)
- · Environmental protection measures
- Exposure must be kept under the limits of the highest expected concentrations (see under "Exposure estimation")
- · Exposure estimation
- Worker (dermal) The highest expected concentration of dermal exposure is ≤ 0.00172 mg/kg bw/d. (PROC 21; RCR 0.101)
- Worker (inhalation) The highest expected concentration of inhalative exposure is ≤ 0.01 mg/m3. (PROC 21; RCR 0.149) Environment
- Estimated/calculated release into the environment (freshwater) after risk management measures: 0.09 kg/d (ERC 10a, 11a) Estimated/calculated release into the environment (air) after risk management measures: 0.5 kg/d (ERC 10a, 11a) Estimated/calculated release into the environment (soil) after risk management measures (a): 3.2 (ERC 10a) Estimated/calculated release into the environment (soil) after risk management measures (b): 0 (ERC 11a) The highest expected concentration for the environmental exposition (local PEC) of freshwater is 0.007 mg/L. (ERC 10a, 11a; RCR 0.280)

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# Trade name: 4-tert-butylbenzoic acid (PTBBA)

(Contd. of page 20) The highest expected concentration for the environmental exposition (local PEC) of freshwater sediment is 0.028 mg/kg dry weight. (ERC 10a, 11a; RCR 0.937) The highest expected concentration for the environmental exposition (local PEC) of marine water is 0.000669 mg/L. (ERC 10a, 11a; RCR 0.279) The highest expected concentration for the environmental exposition (local PEC) of marine water sediment is 0.003 mg/kg dry weight. (ERC 10a, 11a; RCR 0.934) The highest expected concentration for the environmental exposition (local PEC) of STP effluent is 0.045 mg/L. (ERC 10a, 11a; RCR 0.001) The highest expected concentration for the environmental exposition (local PEC) of agricultural soil is 0.000872 mg/kg dry weight. (ERC 10a, 11a; RCR 0.119) **Guidance for downstream users** Risk assessment tool(s) utilised: EUSES version 2.1 ECETOC TRA workers version 3

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# Trade name: 4-tert-butylbenzoic acid (PTBBA)

## Annex: Exposure scenario 5

- Short title of the exposure scenario Use of resin products containing PTBBA (article service life, consumers and professionals)
   Sector of Use
- SU21 Consumer uses: Private households / general public / consumers
- SU22 Professional uses: Public domain (administration, education, entertainment, services, craftsmen)
- · Article category AC13 Plastic articles
- · Environmental release category
- ERC10a Wide dispersive outdoor use of long-life articles and materials with low release
- ERC11a Wide dispersive indoor use of long-life articles and materials with low release
- Physical parameters
- · Physical state
- Solid
- Powder

The substance is present in processed form in articles/products in all ACs.

- · Used amount per time or activity
- $\leq$  500 tons per year and site (ERC 10a, 11a)
- $\leq$  1 tonnes per day and site (a) ERC 10a, 11a)
- · Other operational conditions
- Other operational conditions affecting environmental exposure Receiving surface water flow rate: ≥ 18000 m3/d

Municipal sewage treatment plant (STP)

Discharge rate of sewage treatment plant (STP):  $\geq$  2000 m3/d

application of the STP sludge on agricultural soil

Remark: The given amounts in m3/d refer to a single ERC respectively.

Other operational conditions affecting consumer exposure

Highest product ingredient fraction by weight: 0.001 (for: AC 13, subcategory, plastic, larger articles (plastic chair, PVC-flooring, lawn mower, PC)

Highest product ingredient fraction by weight: 0.001 (for: AC 13, subcategory, toys (doll, car, animals, teething rings)

Highest product ingredient fraction by weight: 0.001 (for: AC 13, subcategory, plastic, small articles (ball pen, mobile phone) Articles/products that are used by consumers may also be used by professionals. This group may therefore also be affected by exposition to the substance.

#### Exposure estimation

#### Environment

Estimated/calculated release into the environment (freshwater) after risk management measures: 0.09 kg/d (ERCs ) Estimated/calculated release into the environment (air) after risk management measures: 0.5 kg/d (ERCs 10a, 11a) Estimated/calculated release into the environment (soil) after risk management measures (a): 3.2 (ERC 10a) Estimated/calculated release into the environment (soil) after risk management measures (b): 0 (ERC 11a) The highest expected concentration for the environmental exposition (local PEC) of freshwater is 0.007 mg/L. (ERC 10a, 11a; RCR

0.280) The highest expected concentration for the environmental exposition (local PEC) of freshwater sediment is 0.028 mg/kg dry weight.

(ERC 10a, 11a; RCR 0.937)

The highest expected concentration for the environmental exposition (local PEC) of marine water is 0.000669 mg/L. (ERC 10a, 11a; RCR 0.279)

The highest expected concentration for the environmental exposition (local PEC) of marine water sediment is 0.003 mg/kg dry weight. (ERC 10a, 11a; RCR 0.934)

The highest expected concentration for the environmental exposition (local PEC) of STP effluent is 0.045 mg/L. (ERC 10a, 11a; RCR 0.001)

The highest expected concentration for the environmental exposition (local PEC) of agricultural soil is 0.000872 mg/kg dry weight. (ERC 10a, 11a; RCR 0.119)

Consumer

The highest expected dermal exposition of consumers is 0.146 mg/kg/d (for: AC 13, subcategory, plastic, larger articles (plastic chair, PVC-flooring, lawn mower, PC))

The highest expected dermal exposition of consumers is 0.0557 mg/kg/d (for: AC 13, subcategory, toys (doll, car, animals, teething rings)



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(Contd. of page 22) The highest expected dermal exposition of consumers is 0.000595 mg/kg/d (for: AC 13, subcategory, plastic, small articles (ball pen, mobile phone))

An oral exposition of consumers is not expected. (for: AC 13, subcategory, plastic, larger articles (plastic chair, PVC-flooring, lawn mower, PC))

The highest expected oral exposition of consumers is 0.001 mg/kg/d (for: AC 13, subcategory, toys (doll, car, animals, teething rings))

The highest expected oral exposition of consumers is 0.00167 mg/kg/d (for: AC 13, subcategory, plastic, small articles (ball pen, mobile phone))