Salts of p-tert-butylbenzoic acid: Human health tier II assessment

30 June 2017

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Chemicals in this assessment

Chemical Name in the Inventory	CAS Number
Benzoic acid, 4-(1,1-dimethylethyl)-, zinc salt	4980-54-5
Benzoic acid, 4-(1,1-dimethylethyl)-, barium salt	10196-68-6
Benzoic acid, 4-(1,1-dimethylethyl)-, calcium salt	52509-84-9
Benzoic acid, 4-(1,1-dimethylethyl)-, zinc salt, basic	101012-86-6

Preface

This assessment was carried out by staff of the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) using the Inventory Multi-tiered Assessment and Prioritisation (IMAP) framework.

The IMAP framework addresses the human health and environmental impacts of previously unassessed industrial chemicals listed on the Australian Inventory of Chemical Substances (the Inventory).

The framework was developed with significant input from stakeholders and provides a more rapid, flexible and transparent approach for the assessment of chemicals listed on the Inventory.

Stage One of the implementation of this framework, which lasted four years from 1 July 2012, examined 3000 chemicals meeting characteristics identified by stakeholders as needing priority assessment. This included chemicals for which NICNAS

already held exposure information, chemicals identified as a concern or for which regulatory action had been taken overseas, and chemicals detected in international studies analysing chemicals present in babies' umbilical cord blood.

Stage Two of IMAP began in July 2016. We are continuing to assess chemicals on the Inventory, including chemicals identified as a concern for which action has been taken overseas and chemicals that can be rapidly identified and assessed by using Stage One information. We are also continuing to publish information for chemicals on the Inventory that pose a low risk to human health or the environment or both. This work provides efficiencies and enables us to identify higher risk chemicals requiring assessment.

The IMAP framework is a science and risk-based model designed to align the assessment effort with the human health and environmental impacts of chemicals. It has three tiers of assessment, with the assessment effort increasing with each tier. The Tier I assessment is a high throughput approach using tabulated electronic data. The Tier II assessment is an evaluation of risk on a substance-by-substance or chemical category-by-category basis. Tier III assessments are conducted to address specific concerns that could not be resolved during the Tier II assessment.

These assessments are carried out by staff employed by the Australian Government Department of Health and the Australian Government Department of the Environment and Energy. The human health and environment risk assessments are conducted and published separately, using information available at the time, and may be undertaken at different tiers.

This chemical or group of chemicals are being assessed at Tier II because the Tier I assessment indicated that it needed further investigation.

For more detail on this program please visit:**www.nicnas.gov.au**

Disclaimer

ACRONYMS & ABBREVIATIONS

Grouping Rationale

This group of four chemical compounds consists of salts of p-tert-butylbenzoic acid (CAS No. 98-73-7). These salts have been included in this group as the physio-chemical properties will not vary greatly and, therefore lead to the compounds within this group having related end uses. The toxicity is considered to result entirely from the parent compound.

The toxic properties of the parent compound, p-tert-butylbenzoic acid (CAS No. 98-73-7) have been assessed as Tier II Inventory Multi-tiered Assessment and Prioritisation (IMAP) assessment (NICNAS). The cations calcium and zinc are considered to be of low systemic toxicity (see IMAP Tranche One—Identification of chemicals of low concern to human health, NICNASa and NICNASb). The barium cation (Ba^{2+}) is reported to be toxic to humans at high doses (ATSDR, 2007), but the toxicological properties of the anion are expected to limit exposure to the barium cation. In the absence of data on chemicals in this group, data for p-tert-butylbenzoic acid are used as 'read-across'.

Import, Manufacture and Use

Australian

The chemical, zinc p-t-butylbenzoate (CAS No. 4980-54-5) has reported commercial use in printing inks. No specific Australian use, import, or manufacturing information has been identified for the rest of the group.

International

The following international uses have been identified through Galleria Chemica; the Substances and Preparations in Nordic countries (SPIN) database; the US Environmental Protection Agency's Aggregated Computer Toxicology Resource (ACToR); the US National Library of Medicine's Hazardous Substances Data Bank (HSDB); the European Union Risk Assessment Report (EU RAR, 2009) and NICNAS assessment report on p-tert-butylbenzoate (NICNAS).

The chemicals have reported commercial use as process regulators in polymers.

The chemicals have reported site-limited use as stabilisers in processing of plasticised PVC.

Restrictions

Australian

No known restrictions have been identified.

International

The chemicals, zinc p-t-butylbenzoate and zinc butylbenzoate basic, are listed on the Health Canada List of prohibited and restricted cosmetic ingredients (The Cosmetic Ingredient ‘Hotlist’)(Galleria Chemica).

No specific international restrictions have been identified for barium p-t-butylbenzoate and calcium p-t-butylbenzoate.

Existing Worker Health and Safety Controls

Hazard Classification

The chemicals are not listed on the Hazardous Chemicals Information System (HCIS) (Safe Work Australia).

Exposure Standards

Australian

No specific exposure standards are available.

International

The following exposure standards are identified for barium p-t-butylbenzoate (Galleria Chemica).

An exposure limit of 0.5 mg/m^3 time weighted average (TWA) in different countries such as the Greece, Hungary, Norway and Russia.

No specific exposure standards are available for other chemicals in the group.

Health Hazard Information

No specific toxicity data are available for these chemicals.

The health hazard information for the parent chemical, p-t-butylbenzoate (CAS No. 98-73-7) is relevant to all chemicals (salts of the parent compound) in this group.

The parent chemical is classified for acute toxicity (harmful), repeated dose toxicity and reproductive and developmental toxicity. The main effects are observed in the central nervous system, liver, kidneys, urinary tract and particularly, the male reproductive system at the concentration range of 17.5–60 mg/kg bw/day. Based on the hazard classification for the parent compound, these chemicals also warrant hazard classification (see **Recommendation** section).

The Tier II assessment for the parent chemical is available at: **https://www.nicnas.gov.au/chemical-information/imap-assessments/imap-assessment-details?assessment_id=873**. The report should be read in conjunction with this Tier II assessment.

Risk Characterisation

Critical Health Effects

Based on information for the parent chemical, p-t-butylbenzoate (CAS No. 98-73-7) (NICNAS), chemicals in this group are considered to have systemic long-term effects (reproductive toxicity and serious damage to health following repeated exposure regardless of the route of exposure). The critical health effects for risk characterisation also include systemic acute toxicity from oral exposure.

Public Risk Characterisation

Given the uses identified for the chemicals internationally, it is unlikely that the public will be exposed. Although the public could come into contact with articles or coated surfaces containing the chemicals, it is expected that the chemicals will be bound within the article or coated surface and hence will not be bioavailable. Therefore, the chemicals are not considered to pose an unreasonable risk to public health. Should information become available to indicate cosmetic or domestic use of these chemicals, further regulatory controls may be required.

The parent chemical was recommended for Tier III assessment to determine whether the chemical is used in cosmetic and domestic products in Australia (NICNAS). The salts in this assessment should be considered as part of this Tier III.

Occupational Risk Characterisation

During product formulation, oral, dermal and inhalation exposure may occur, particularly where manual or open processes are used. These could include transfer and blending activities, quality control analysis, and cleaning and maintaining equipment. Worker exposure to the chemicals at lower concentrations could also occur while using formulated products containing the chemicals. The level and route of exposure will vary depending on the method of application and work practices employed.

Given the critical systemic long-term health effects, the chemicals could pose an unreasonable risk to workers unless adequate control measures to minimise oral, dermal and inhalation exposure are implemented. The chemicals should be appropriately classified and labelled to ensure that a person conducting a business or undertaking (PCBU) at a workplace (such as an employer) has adequate information to determine the appropriate controls.

The data available support an amendment to the hazard classification in the HCIS (Safe Work Australia) (see **Recommendation** section).

A risk assessment conducted internationally for the parent chemical (EURAR, 2009) concluded that, for two occupational exposure scenarios: (1) production and further processing of PTBBA (2) production of alkyd resins in the polymers industry, 'there is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account' (EURAR, 2009). A recommendation was made for Safe Work Australia to consider whether current controls are adequate to minimise the risk to workers (NICNAS). The salts in this assessment should be considered as part of this process.

NICNAS Recommendation

Safe Work Australia should consider whether current controls are adequate to minimise the risk to workers. A Tier III assessment may be necessary to provide further information as to whether the current exposure controls are appropriate to offer adequate protection to workers. In addition, the chemical is recommended for Tier III assessment to determine whether the chemical is used in cosmetic and domestic products in Australia. If the chemical is used in this country, a quantitative risk assessment should be undertaken to characterise the risk.

All other risks are considered to have been sufficiently assessed at the Tier II level, provided that the recommended amendment to the classification is adopted, and labelling and all other requirements are met under workplace health and safety and poisons legislation as adopted by the relevant state or territory.

Regulatory Control

Work Health and Safety

The chemicals are recommended for classification and labelling aligned with the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) as below. This does not consider classification of physical hazards and environmental hazards.

From 1 January 2017, under the model Work Health and Safety Regulations, chemicals are no longer to be classified under the Approved Criteria for Classifying Hazardous Substances system.

Hazard	Approved Criteria (HSIS)[a]	GHS Classification (HCIS)[b]
Acute Toxicity	Not Applicable	Harmful if swallowed - Cat. 4 (H302)
Repeat Dose Toxicity	Not Applicable	Causes damage to organs through prolonged or repeated exposure - Cat. 1 (H372)
Reproductive and Developmental Toxicity	Not Applicable	May damage fertility - Cat. 1B (H360F)

[a] Approved Criteria for Classifying Hazardous Substances [NOHSC:1008(2004)].

[b] Globally Harmonized System of Classification and Labelling of Chemicals (GHS) United Nations, 2009. Third Edition.

[*] Existing Hazard Classification. No change recommended to this classification

Advice for industry

Control measures

Control measures to minimise the risk from oral, dermal and inhalation exposure to the chemicals should be implemented in accordance with the hierarchy of controls. Approaches to minimise risk include substitution, isolation and engineering controls. Measures required to eliminate, or minimise risk arising from storing, handling and using a hazardous chemical depend on the physical form and the manner in which the chemicals are used. Examples of control measures that could minimise the risk include, but are not limited to:

- using closed systems or isolating operations;

- using local exhaust ventilation to prevent the chemicals from entering the breathing zone of any worker;
- health monitoring for any worker who is at risk of exposure to the chemicals, if valid techniques are available to monitor the effect on the worker's health;
- air monitoring to ensure control measures in place are working effectively and continue to do so;
- minimising manual processes and work tasks through automating processes;
- work procedures that minimise splashes and spills;
- regularly cleaning equipment and work areas; and
- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with the chemicals.

Guidance on managing risks from hazardous chemicals are provided in the *Managing risks of hazardous chemicals in the workplace—Code of practice* available on the Safe Work Australia website.

Personal protective equipment should not solely be relied upon to control risk and should only be used when all other reasonably practicable control measures do not eliminate or sufficiently minimise risk. Guidance in selecting personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

Obligations under workplace health and safety legislation

Information in this report should be taken into account to help meet obligations under workplace health and safety legislation as adopted by the relevant state or territory. This includes, but is not limited to:

- ensuring that hazardous chemicals are correctly classified and labelled;
- ensuring that (material) safety data sheets ((M)SDS) containing accurate information about the hazards (relating to both health hazards and physicochemical (physical) hazards) of the chemicals are prepared; and
- managing risks arising from storing, handling and using a hazardous chemical.

Your work health and safety regulator should be contacted for information on the work health and safety laws in your jurisdiction.

Information on how to prepare an (M)SDS and how to label containers of hazardous chemicals are provided in relevant codes of practice such as the *Preparation of safety data sheets for hazardous chemicals—Code of practice* and *Labelling of workplace hazardous chemicals—Code of practice*, respectively. These codes of practice are available from the Safe Work Australia website.

A review of the physical hazards of these chemicals has not been undertaken as part of this assessment.

References

Agency for Toxic Substances and Disease Registry (ATSDR) 2007. Toxicological Profile for Barium and Barium Compounds. U.S. Department of Health and Human Services. Available at **http://www.atsdr.cdc.gov/toxprofiles/tp24.pdf**

Galleria Chemica. Accessed November 2016 at **http://jr.chemwatch.net/galleria/**

Globally Harmonised System of Classification and Labelling of Chemicals (GHS) United Nations, 2009. Third edition. Accessed at **http://www.unece.org/trans/danger/publi/ghs/ghs_rev03/03files_e.html**

National Industrial Chemicals Notification and Assessment Scheme (NICNAS). Human health Tier II assessment for benzoic acid, 4-(1,1-dimethylethyl)- (CAS No. 98-73-7). Australian Government Department of Health. Accessed December 2016 at **https://www.nicnas.gov.au**

National Industrial Chemicals Notification and Assessment Scheme (NICNASa). Identification of chemicals of low concern to human health. Available at **http://www.nicnas.gov.au**

National Industrial Chemicals Notification and Assessment Scheme (NICNASb). Human health Tier II assessment for soluble zinc salts. Accessed February 2017 at **https://www.nicnas.gov.au/**

Safe Work Australia. Hazardous Chemicals Information System (HCIS). Accessed January 2017 at **http://hcis.safeworkaustralia.gov.au/HazardousChemical**

Substances in Preparations in Nordic Countries (SPIN) Database. Accessed November 2016 at **http://spin2000.net/**

The US Environmental Protection Agency (EPA) Aggregated Computer Toxicology Resource (ACToR) database. Accessed November 2016 at **http://actor.epa.gov/actor/faces/ACToRHome.jsp**

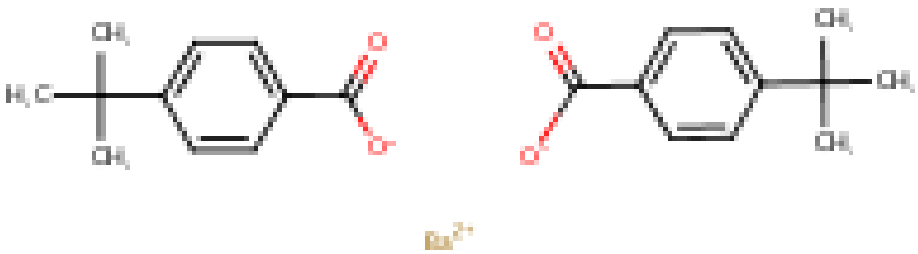
United States (US) National Library of Medicine's Hazardous Substances Data Bank (HSDB). Accessed November 2016 at **http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB**

Last Update 30 June 2017

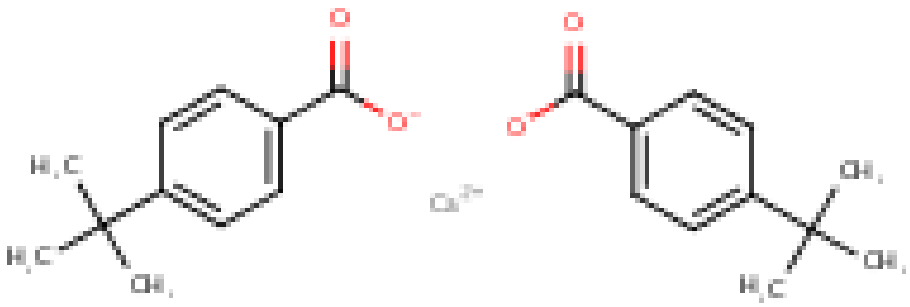
Chemical Identities

Chemical Name in the Inventory and Synonyms	**Benzoic acid, 4-(1,1-dimethylethyl)-, zinc salt** zinc p-t-butylbenzoate
CAS Number	4980-54-5
Structural Formula	
Molecular Formula	C11H14O2.1/2Zn

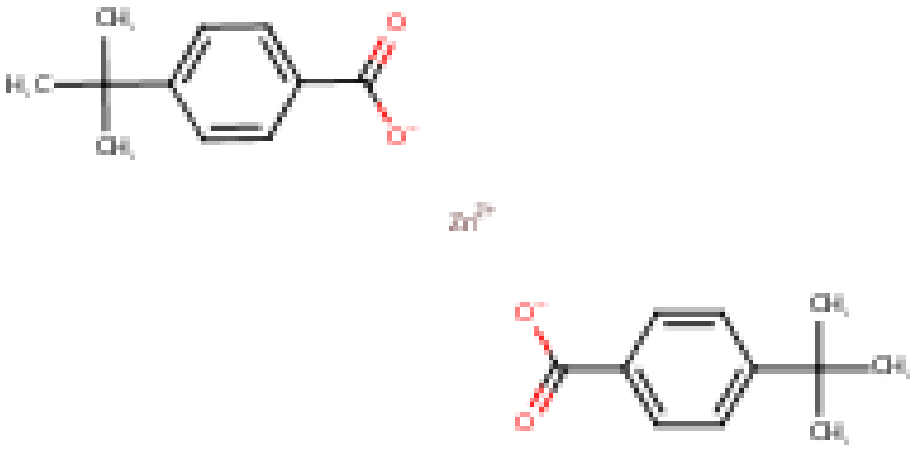
Molecular Weight	419.8

Chemical Name in the Inventory and Synonyms	**Benzoic acid, 4-(1,1-dimethylethyl)-, barium salt** barium p-t-butylbenzoate
CAS Number	10196-68-6
Structural Formula	
Molecular Formula	C11H14O2.1/2Ba
Molecular Weight	491.7

Chemical Name in the Inventory and Synonyms	**Benzoic acid, 4-(1,1-dimethylethyl)-, calcium salt** calcium p-t-butylbenzoate p-tert-butylbenzoic acid, calcium salt
CAS Number	52509-84-9

Structural Formula	
Molecular Formula	C11H14O2.1/2Ca
Molecular Weight	394-5

Chemical Name in the Inventory and Synonyms	**Benzoic acid, 4-(1,1-dimethylethyl)-, zinc salt, basic** zinc butyl benzoate, basic
CAS Number	101012-86-6
Structural Formula	

	
Molecular Formula	Unspecified
Molecular Weight	419.8

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