Phenol, 2,4,6-tris(1,1-dimethylethyl)-: Environment tier II assessment

11 April 2014

CAS Registry Number: 732-26-3.

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.

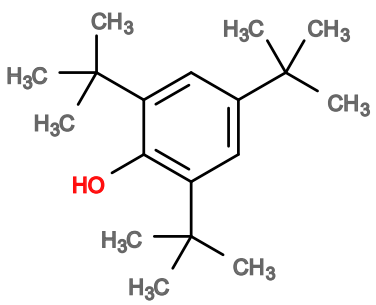
This chemical or group of chemicals are being assessed at Tier II because the Tier I assessment indicated that it needed further investigation.

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

Disclaimer

Acronyms & Abbreviations

Chemical Identity

Synonyms	2,4,6-Tri-*tert*-butylphenol
Structural Formula	
Molecular Formula	$C_{18}H_{30}O$

Molecular Weight (g/mol)	262.43
SMILES	C(C)(C)(C)c1c(O)c(C(C)(C)C)cc(C(C)(C)C)c1

Physical and Chemical Properties

The physical and chemical property data for phenol, 2,4,6-tris(1,1-dimethylethyl)- (or 2,4,6-tri-*tert*-butylphenol) were retrieved from the databases included in the OECD QSAR Toolbox (LMC, 2013).

Physical Form	Solid
Melting Point	131°C (exp.)
Boiling Point	278°C (exp.)
Vapour Pressure	0.088 Pa (exp.)
Water Solubility	35 mg/L (exp.)
Ionisable in the Environment?	No
log K_{ow}	6.06 (exp.)

Import, Manufacture and Use

Australia

No specific Australian use, import, or manufacturing information has been identified.

International

The chemical is used in aviation gasolines as an antioxidant and is the starting material for the synthesis of 2,6-di-*tert*-butyl-4-methoxyphenol (US NLM, 2013). In the calendar year 2005, 10 million to 50 million pounds [4536 tonnes to 22 680 tonnes] of the chemical was produced and/or imported in the United States (US EPA, 2009).

According to the Canadian authorities, the primary end-use application of 2,4,6-tri-*tert*-butylphenol is as an antioxidant in hydrocarbon fuels such as gasoline, jet fuel, diesel and biodiesel (Environment Canada, 2009).

In Europe, an OSPAR Commission Report indicated there was some uncertainty regarding the precise use patterns of the chemical. The only confirmed uses were as a chemical intermediate in the production of antioxidants used in rubber and plastic and in lubricating agents in the transport sector (though it was unknown whether it was an intentional additive or impurity). It may also be a by-product in the production of 4-*tert*-butylphenol (OSPAR, 2006). However, the current REACH dossier for the chemical only lists use as a chemical intermediate (ECHA, 2014a).

In the Nordic countries the chemical is used as an additive in fuels, lubricants (including cutting oils) and hydraulic fluids and as a stabiliser (Nordic Council of Ministers, 2013).

Industrial use of 2,4,6-tri-*tert*-butylphenol is prohibited in Japan (Government of Japan, 2010; NITE, 2014).

Environmental Regulatory Status

Australia

The chemical meets the definition of a Discrete Organic Chemical under the *Chemical Weapons (Prohibition) Act 1994 (Cwlth)*. Production of the chemical in volumes greater than 200 tonnes per annum in Australia must be reported to the Australian Safeguards and Non-Proliferation Office of the Australian Government Department of Foreign Affairs and Trade (DFAT, 2009).

United Nations

The chemical is not currently identified as a Persistent Organic Pollutant (UNEP, 2001), ozone depleting substance (UNEP, 1985), or hazardous substance for the purpose of international trade (UNEP, 1998).

OECD

The chemical is considered a High Production Volume (HPV) chemical by the OECD, which indicates that more than 1000 tonnes of the chemical are used per year in at least one member country (OECD, 2013).

The chemical has not been sponsored for assessment under the Cooperative Chemicals Assessment Programme (CoCAP) (OECD, 2013).

Canada

In a screening assessment the chemical was identified as a high priority for assessment of ecological risk as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms, and known to be in commerce in Canada (Environment Canada, 2008). The final screening assessment report concluded that 2,4,6-tri-*tert*–butylphenol meets the virtual elimination criteria under subsection 77(4) of the *Canadian Environmental Protection Act, 1999*. Chemicals listed on the Virtual Elimination List must not be released to the environment in quantities that result in environmental concentrations above an assigned Level of Quantitation (Environment Canada, 2009).

European Union

The chemical is not listed on the Candidate List for Eventual Inclusion in Annex XIV, Annex XIV (authorisation) or Annex XVII (restriction) of the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation. Therefore, the chemical is not subject to authorisation or restriction, and is not currently identified by the European Union as a substance of very high concern for the environment (ECHA, 2013; 2014b; 2014c).

Japan

In Japan, all uses of the chemical are prohibited except for testing or research purposes. The chemical has been found to be persistent in the environment, bioaccumulative and to pose a risk to human health or the human living environment, and has been classified as a Class I Specified Chemical Substance under the *Act on the Evaluation of Chemical Substances and Regulation of Their Manufacture, etc., 1973* (the Chemical Substances Control Law) (Government of Japan, 2010).

United States of America

This chemical does not belong to any of the chemical classes covered by an Existing Chemical Action Plan and has not been selected for action plan development (US EPA, 2013).

Environmental Exposure

In accordance with the IMAP Framework, it is assumed that up to 100 tonnes of the chemical could be imported and/or manufactured in Australia annually (NICNAS, 2013).

Based on use information from other industrialised countries, the highest volume use of the chemical would be as an additive for hydrocarbon fuels and as a component of industrial lubricants. The use of 2,4,6-tri-*tert*-butylphenol as a fuel additive is expected to result in destruction of this organic chemical through combustion in engines. However, emissions to the environment from other sources such a spills and inappropriate disposal are possible. The use of 2,4,6-tri-*tert*–butylphenol in industrial lubricants has the potential to lead to environmental releases of this chemical based on standard exposure scenarios for lubricants (OECD, 2004).

Environmental Fate

Partitioning

The chemical is expected to mainly partition to the soil and sediment compartments as a result of industrial use.

The chemical is a very weak acid (pK_a = 12.20) (LMC, 2013), which is moderately soluble in water and moderately volatile. The estimated Henry's Law constant for the chemical (0.7-0.9 Pa-m^3/mol) indicates that it is moderately volatile from water and moist soil (US EPA, 2008).

The low dissociation constant of the chemical indicates that it is not expected to be ionised in the environment. The measured octanol-water partitioning constant (log K_{ow} = 6.06) and the estimated soil absorption coefficient (K_{oc} > 10 000 L/kg) are therefore likely to be reliable metrics for predicting partitioning behaviour in the environment. On the basis of these partitioning constants, this chemical can be characterised as a highly lipophilic neutral organic substance that will be immobile in soil.

Calculations with a standard multimedia partitioning (fugacity) model assuming equal and continuous emission of the chemical to the air, water and soil compartments (Level III approach) predict that the majority of the chemical will partition to soil (58.8%) and sediment (33.3%) and lower amounts are predicted to partition to water (7.63%) and air (0.268%) (US EPA, 2008). These calculations do not take into account the combustion of the chemical, if it is used as a fuel additive.

Degradation

The chemical is not expected to degrade rapidly in the environment.

In air, the chemical is predicted to have a half-life of 8 hours due to photo-oxidation by hydroxyl radicals (US EPA, 2008).

Only one biodegradation study was available for the chemical. A biological oxygen demand (BOD) of 0% was reported after 28 days in a study conducted in accordance with OECD Test Guideline (TG) 301 C (LMC, 2013). The chemical is predicted to have a half life of > 6 months for primary biodegradation according to calculations conducted with the CATALOGIC 301C metabolism simulator (LMC, 2011).

No experimental data for degradation in soil or sediment compartments have been identified for the chemical or a suitable analogue. The half lives in soil and sediment for the chemical are estimated to be > 6 months and > 2 years, respectively, based on standard factors for extrapolation of degradation half-lives from biodegradability tests in water (EPHC, 2009).

Bioaccumulation

The chemical is expected to bioaccumulate in aquatic organisms.

The experimental bioconcentration factor (BCF) in fish is reported to range from 4320 to 23 200 L/kg at a test concentration of 1 mg/L and 4830 to 16 000 L/kg at 10 mg/L. Ten fish were tested at each concentration (Environment Canada, 2008). These measured BCF values significantly exceed the domestic categorisation threshold for bioaccumulation of 2000 L/kg.

No experimental data for bioaccumulation in terrestrial or sediment organisms have been identified for the chemical or a suitable analogue.

Transport

Based on its low potential to partition to the atmosphere and predicted rapid degradation in the troposphere by indirect photo-oxidation, the chemical is not expected to undergo long-range transport.

Predicted Environmental Concentration (PEC)

There is currently insufficient information to calculate the PEC of the chemical in the Australian environment. However, based on overseas use patterns, the majority of the introduced chemical would be expected to be combusted in fuels to which it has been added. If the chemical were released to waterways it is expected to mainly partition to sediment. According to the SimpleTreat model (Struijs, 1996), if the chemical was released to sewage treatment plants, the majority (85%) is expected to partition to biosolids which may be applied to agricultural soils. Therefore, the soil and sediment compartments are expected to be most impacted by releases of the chemical to the environment.

Environmental Effects

Effects on Aquatic Life

The chemical is acutely toxic to aquatic organisms at low concentrations.

Acute toxicity

There are measured aquatic ecotoxicological data available for this chemical. The following median lethal concentration (LC50) and median effective concentrations (EC50s) for model organisms across three trophic levels were obtained from databases in the OECD QSAR Toolbox (LMC, 2013) and used to characterise the acute effects of this chemical:

Taxon	Endpoint	Method
Fish	96 h LC50 = 0.0609 mg/L	Experimental *Pimephales promelas* (Fathead minnow) Flow-through
Invertebrates	48 h EC50 = 0.11 mg/L	Experimental *Daphnia magna* (Water flea) OECD TG 202
Algae	72 h EC50 > 0.32 mg/L	Experimental *Pseudokirchneriella subcapitata* (Green algae) OECD TG 201

Chronic toxicity

The following no-observed-effect concentrations (NOECs) for model organisms from two major aquatic trophic levels were obtained from databases included in the OECD QSAR Toolbox (LMC, 2013):

Taxon	Endpoint	Method
Invertebrates	21 d NOEC = 0.36 mg/L	Experimental *Daphnia magna* (Water flea) OECD TG 211
Algae	72 h NOEC = 0.32 mg/L	Experimental *Pseudokirchneriella subcapitata* (Green algae) OECD TG 201

The ecotoxicity data set for this chemical is incomplete as no chronic fish toxicity data are available. This is considered to be a significant gap in the available data for 2,4,6-tri-*tert*-butylphenol because it has a very high bioaccumulation potential in fish.

Effects on Terrestrial Life

No data for effects on terrestrial organisms have been identified for the chemical or a suitable analogue.

Predicted No-Effect Concentration (PNEC)

The chemical is highly bioaccumulative in aquatic organisms and environmentally persistent. These two hazard characteristics combined have the potential to result in a range of long term effects on aquatic life exposed to this chemical which cannot be readily identified through standard toxicity tests. For such chemicals, it is not currently possible to estimate a safe exposure concentration using standard extrapolation methods based on laboratory screening level tests. There is further uncertainty regarding possible long term effects of this chemical resulting from the incomplete set of screening level chronic aquatic toxicity data. A PNEC for the aquatic compartment has therefore not been derived for 2,4,6-tri-*tert*-butylphenol.

Categorisation of Environmental Hazard

The categorisation of the environmental hazards of phenol, 2,4,6-tris(1,1-dimethylethyl)- according to domestic environmental hazard thresholds is presented below (EPHC, 2009; NICNAS, 2013):

Persistence

Persistent (P). Based on a measured BOD of 0% in a standard aerobic biodegradation test the chemical is categorised as Persistent.

Bioaccumulation

Bioaccumulative (B). Based on measured bioconcentration factors ≥ 4320 L/kg the chemical is categorised as Bioaccumulative.

Toxicity

Toxic (T). Based on the measured 96 h LC50 for fish (*P. promelas*) of 0.0609 mg/L the chemical is categorised as Toxic.

Summary

Phenol, 2,4,6-tris(1,1-dimethylethyl)- is categorised as:

- P
- B
- T

Risk Characterisation

The chemical has been identified as a PBT substance. It is not currently possible to derive a safe environmental exposure level for such chemicals and it is therefore not appropriate to characterise the environmental risks for this chemical in terms of a risk quotient.

Due to their persistence, PBT chemicals have the potential to become widely dispersed environmental contaminants. Once in the environment, persistent chemicals that are also bioaccumulative pose an increased risk of accumulating in exposed organisms and of causing adverse effects. They may also biomagnify through the food chain resulting in very high internal concentrations, especially in top predators. Importantly, it is difficult or impossible to reverse the adverse effects of PBT chemicals once they have been released. As a result, these chemicals are considered to be of high concern for the environment.

Key Findings

The chemical is typically used as an antioxidant/stabiliser in hydrocarbon fuels and lubricants. Although industrial uses for this chemical have been identified in other industrialised countries, there is currently no specific information on either the annual volumes of this chemical that are introduced or the industrial use pattern in Australia.

The chemical has been identified as hazardous to the environment by the Governments of Japan and Canada. It is currently prohibited for industrial uses in Japan and has been proposed for virtual elimination under specific risk management plans in Canada.

The present screening level risk assessment has established that 2,4,6-tri-*tert*-butylphenol is a PBT substance according to domestic environmental hazard criteria and is therefore considered a high concern substance.

A key component of effective risk reduction measures for PBT chemicals is to identify the routes of potential environmental exposure and the quantities of chemicals entering the environment by various exposure pathways. Currently, this analysis cannot be conducted in Australia due to the lack of essential exposure information including introduction volumes and industrial uses. These are critical data gaps in the risk profile for the industrial uses of this chemical in Australia.

This chemical may need to be prioritised for a Tier III risk assessment under the IMAP framework. The specific focus of such an assessment would be a consideration of the environmental exposure resulting from industrial uses of 2,4,6-tri-*tert*-butylphenol in Australia, and the effectiveness of current risk management measures for this chemical.

Recommendations

It is recommended that phenol, 2,4,6-tris(1,1-dimethylethyl)- be considered for assessment of environmental concerns at Tier III level under the IMAP framework.

Environmental Hazard Classification

In addition to the categorisation of environmental hazards according to domestic environmental thresholds presented above, the classification of the environmental hazards of phenol, 2,4,6-tris(1,1-dimethylethyl)- according to the third edition of the United Nations' Globally Harmonised System of Classification and Labelling of Chemicals (GHS) is presented below (UNECE, 2009):

Hazard	GHS Classification (Code)	Hazard Statement
Acute Aquatic	Category 1 (H400)	Very toxic to aquatic life
Chronic Aquatic	Category 1 (H410)	Very toxic to aquatic life with long lasting effects

The chemical has been classified as Aquatic Chronic 1 according to the most stringent outcome method of the GHS for long-term aquatic hazard classification of chemical substances. The classification is based on the measured acute fish toxicity data for phenol, 2,4,6-tris(1,1-dimethylethyl)- taking into account the persistence and bioaccumulation properties of the chemical.

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