Australian Government
Department of Health
Australian Industrial Chemicals Introduction Scheme

2-Phenylphenol and salts

Evaluation statement

30 May 2022

Table of contents

Contents

AICIS evaluation statement

Subject of the evaluation

2-Phenylphenol and salts

Chemicals in this evaluation

Name	CAS registry number
[1,1'-Biphenyl]-2-ol	90-43-7
[1,1'-Biphenyl]-2-ol, sodium salt	132-27-4
[1,1'-Biphenyl]-2-ol, sodium salt, tetrahydrate	6152-33-6
[1,1'-Biphenyl]-2-ol, potassium salt	13707-65-8

Reason for the evaluation

Evaluation Selection Analysis indicated a potential environmental risk.

Parameters of evaluation

This evaluation considers the environmental risks associated with the industrial use of [1,1'-biphenyl]-2-ol, hereinafter referred to as 2-phenylphenol (2PP), and its sodium (S2PP) and potassium (P2PP) salts. This group of chemicals has been assessed for risks to the environment according to the following parameters:

- default imported volumes of 100 tonnes per annum each for 2-phenylphenol and both forms of the sodium salt
- a notified volume of up to 100 tonnes per annum for the potassium salt
- industrial uses listed in the ‘Summary of Use’ section
- expected release primarily to sewage treatment plants (STPs) from their industrial uses.

Chemicals in this evaluation have been assessed as a group as they have similar use patterns and will all form the same chemical species (2-phenylphenol) under normal environmental conditions. The environmental risks of the sodium and potassium cations of the corresponding salts in this evaluation are not considered, as they are either ubiquitous in the environment or have previously been assessed.

Summary of evaluation

Summary of introduction, use and end use

2-Phenylphenol is a high production volume chemical with a complex variety of industrial and other uses. No information on domestic introduction volumes is available for 2-phenylphenol

or the sodium salt and its tetrahydrate. The potassium salt of 2-phenylphenol has previously been assessed for introduction in Australia as a preservative in water based products used in paper manufacture at volumes of 30–100 tonnes/year (NICNAS 2006). The other chemicals are each assumed to be used at the default domestic introduction volume of 100 tonnes/year.

This group of chemicals has been assessed for use as biocides, preservatives, and intermediates in the following industrial products:

- adhesive and sealant products
- apparel and footwear care products
- arts, crafts, and hobby products
- fuel, oil, fuel oil additives and related products
- lubricant and grease products
- personal care products – limited environmental release
- paint and coating products
- plastic and polymer products
- construction products not covered by other end uses
- ink, toner, and colourant products
- air care products
- automotive care products
- cleaning and furniture care products
- laundry and dishwashing products
- paper products
- personal care products not covered by other end uses
- any other end use not covered above (e.g., intermediate).

Environment

Summary of environmental hazard characteristics

According to domestic environmental hazard thresholds and based on the available data chemicals in this group are:

- Not Persistent (not P)
- Not Bioaccumulative (not B)
- Toxic (T).

There is some evidence to suggest that these chemicals may cause some endocrine mediated effects in fish.

Environmental hazard classification

These chemicals satisfy the criteria for classification according to Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (UNECE 2017). The classification of the acute and chronic aquatic hazards posed by these chemicals was performed based on the measured ecotoxicity data presented in this evaluation. This evaluation does not consider classification of physical hazards and health hazards:

Environmental Hazard	Hazard Category	Hazard Statement
Acute Aquatic	Acute Aq. – Cat. 2	H401: Toxic to aquatic life
Chronic Aquatic	Chronic Aq. – Cat. 1	H410: Very toxic to aquatic life with long lasting effects

Summary of environmental risk

2-Phenylphenol and its salts are readily biodegradable and have low bioaccumulation potential. These chemicals exhibit acute and significant chronic toxicity and some potential to cause endocrine mediated effects in fish. They are classified as very toxic to aquatic life with long lasting effects.

Based on measured and predicted concentrations in Australian surface waters, and Australian and international sewage treatment plant effluent and biosolids, 2-phenylphenol and its salts are not expected to pose a significant risk to the Australian environment as environmental concentrations are below the levels likely to cause harmful effects.

There is evidence to suggest that these chemicals may cause some endocrine mediated effects. Although some uncertainty remains, the available information indicates that significant endocrine effects are not expected at the predicted environmental concentrations or at levels below which other toxic effects occur.

Conclusions

The conclusions of this evaluation are based on the information described in this Evaluation statement.

The Executive Director is satisfied that the identified environment risks can be managed within existing risk management frameworks. This is provided that all requirements are met under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory.

Note: Obligations to report additional information about hazards under *Section 100 of the Industrial Chemicals Act 2019* apply. In addition, for CAS No. 13707-65-8 obligations apply to provide any information specifically required by the terms of the Inventory listing under *Section 101, of the Industrial Chemicals Act 2019.*

Supporting information

Rationale

This evaluation considers the environmental risks associated with the industrial use of [1,1'-biphenyl]-2-ol, hereinafter referred to as 2-phenylphenol (2PP), and its salts. Chemicals in this group are used in high volumes internationally and were selected for evaluation because the Evaluation Selection Analysis indicated a potential risk to the environment. Chemicals in this evaluation have been assessed as a group as they have similar use patterns and will all form the same chemical species (2-phenylphenol) under normal environmental conditions.

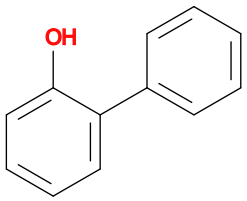
The potassium salt of 2-phenylphenol (P2PP) was previously assessed as a new chemical under the former, *Industrial Chemical (Notification and Assessment) Act* 1989, and subsequently added to the Australian Inventory of Industrial Chemicals (NICNAS 2006). This chemical is included in this evaluation due to new information about the possible endocrine effects of 2PP and its salts.

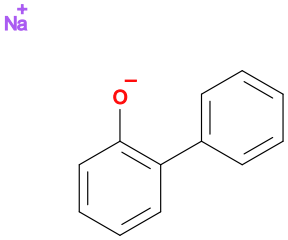
Chemical identity

This evaluation considers 2-phenylphenol (2PP, CAS No. 90-43-7), and its potassium and sodium salts and hydrates listed on the Australian Inventory of Industrial Chemicals.

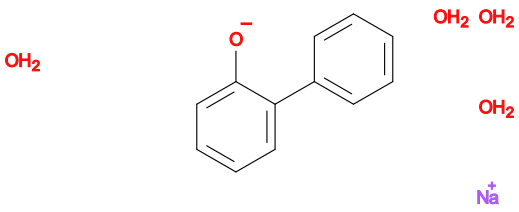
The chemical 2-phenylphenol is prepared by auto-condensation of cyclohexanone to give 2-cyclohexenylcyclohexanone, which is subsequently dehydrogenated to 2PP (Fiege et al. 2012). As a weak acid, 2PP reacts with strong bases (e.g., NaOH, KOH) to form salts that are soluble in water (Weber et al. 2012). The sodium salt and its tetrahydrate (S2PP, CAS Nos. 132-27-4 and 6152-33-6, respectively) and the potassium salt (P2PP, CAS No. 13707-65-8) are formed in this way:

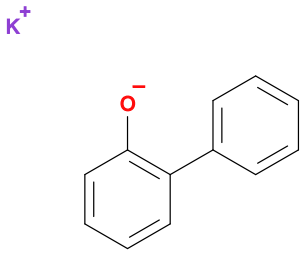
Chemical name	[1,1'-Biphenyl]-2-ol
CAS No.	90-43-7
Synonyms	2-phenylphenol (2PP) orthophenylphenol (OPP) 2-biphenylol o-phenylphenol biphenyl-2-ol 2-hydroxybiphenyl o-xenol Trade names include Dowicide, Torsite, Preventol, Nipacide and Lysol (NCBIa).

Structural formula	
Molecular formula	$C_{12}H_{10}O$
Molecular weight (g/mol)	170.21
SMILES	C1=CC=C(C=C1)C2=CC=CC=C2O
Chemical description	-

Chemical name	[1,1'-Biphenyl]-2-ol, sodium salt
CAS No.	132-27-4
Synonyms	2-phenylphenol sodium salt (S2PP) sodium [1,1'-biphenyl]-2-olate sodium 2-biphenylate sodium o-phenylphenate sodium o-phenylphenoxide 2-hydroxybiphenyl, sodium salt
Structural formula	
Molecular formula	$C_{12}H_9O.Na$
Molecular weight (g/mol)	192.19
SMILES	C1=CC=C(C=C1)C2=CC=CC=C2[O-].[Na+]
Chemical description	-

Chemical name	[1,1'-Biphenyl]-2-ol, sodium salt, tetrahydrate
CAS No.	6152-33-6

Synonyms	2-phenylphenol sodium salt tetrahydrate (S2PP) o-Phenylphenol, sodium salt, tetrahydrate sodium [1,1'-biphenyl]-2-olate tetrahydrate sodium 2-biphenylate tetrahydrate sodium o-phenylphenate tetrahydrate sodium o-phenylphenoxide tetrahydrate
Structural formula	
Molecular formula	$C_{12}H_9O.4H_2O.Na$
Molecular weight (g/mol)	264.25
SMILES	C1=CC=C(C=C1)C2=CC=CC=C2[O-].O.O.O.O.[Na+]
Chemical description	-

Chemical name	[1,1'-Biphenyl]-2-ol, potassium salt
CAS No.	13707-65-8
Synonyms	2-phenylphenol potassium salt (P2PP) potassium [1,1'-biphenyl]-2-olate potassium 2-biphenylate potassium o-phenylphenate potassium o-phenylphenoxide 2-hydroxybiphenyl, potassium salt
Structural formula	
Molecular formula	$C_{12}H_9O.K$
Molecular weight (g/mol)	208.30
SMILES	C1=CC=C(C=C1)C2=CC=CC=C2[O-].[K+]
Chemical description	-

Relevant physical and chemical properties

Measured physical and chemical property data for 2-phenylphenol were retrieved from the databases included in the Organisation for Economic Co-operation and Development (OECD) QSAR Toolbox (LMC 2021) and dossiers submitted under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation in the European Union (EU) (REACHb). The Henry's Law constant was calculated from the measured values for water solubility and vapour pressure using EPISuite (US EPA 2017):

Chemical	2-phenylphenol (2PP)
Physical form	Solid
Melting point	59°C (exp. database)
Boiling point	286°C (exp. database)
Vapour pressure	0.474 Pa at 20°C (exp.)
Water solubility	0.560 g/L at 20°C (exp.)
Henry's Law constant	0.14 $Pa \cdot m^3/mol$ (calc.)
Ionisable in the environment?	No
pKa	9.5 at 20°C (exp.)
log K_{OW}	3.18 at 22.5°C (exp.)

Compared to the parent chemical, the sodium and potassium salts of 2-phenylphenol are much more water soluble. The hydrated sodium salt has a higher vapour pressure due to bound water. However, in the aqueous environment, these chemicals are in pH dependent equilibrium and the salts will rapidly dissociate and form 2-phenylphenol (the free acid) as the dominant form in the environmentally relevant pH range (pH = 4–9).

Introduction and use

Australia

No specific Australian use information has been identified for 2PP or S2PP. In 2006, P2PP was assessed in Australia as a new chemical with a maximum introduction volume of 30–100 tonnes/year over the following 5 years. It is used as a preservative in water based products used in paper manufacture (NICNAS 2006).

International

2-Phenylphenol is listed by the OECD as a high production volume chemical indicating an international use volume of more than 1 000 t/year (OECD 2009, n.d.). It is also listed as a high production volume chemical in the United States of America, indicating it is produced or imported there in quantities exceeding 1 million pounds per year (about 500 t/year) (US

EPAa). In the European Union, 2PP and S2PP are each used in the range of 10 to 100 t/year (REACHa; REACHb). In the Nordic countries, the average annual use volume over the 5 year period from 2015–2019 was about 9 t/year (SPIN). In Japan, manufactured and imported quantities ranged from 1000–6000 t/year between 2015–2019 (NITE). The quantity range is 1–1000 t/year on the Domestic Substances List in Canada (ECCC).

As reported in previous Australian assessments (NICNAS 2006; 2015), the following international uses have been identified through:

- the European Union REACH dossiers (REACHa; REACHb)
- the European Commission's Cosmetic Substances and Ingredients (CosIng) database (EC)
- Galleria Chemica (Chemwatch)
- the Haz-Map occupational health database (Haz-Map)
- the Substances and Preparations in Nordic countries database (SPIN)
- the Personal Care Products Council's International Cosmetic Ingredient Dictionary and Handbook (PCPC)
- the US National Library of Medicine's Hazardous Substances Data Bank (NCBIb)
- various international assessments (CEPA 2007; 2016; German Research Foundation 2020; IARC 1999; INCHEM 1999).

Chemicals in this group have the following reported cosmetics uses:

- as cosmetic preservatives
- in hair colouring preparations
- as ingredients in fragrances
- as ingredients in cleansing products such as cold creams, cleansing lotions, liquids, pads, and in mud pack pastes.

Chemicals in this group have one or more of the following reported uses in consumer products:

- in lubricants and additives
- as preservatives in cleaning/washing agents
- as preservatives in food packaging
- in paints, lacquers, and varnishes
- in aerosol disinfectant products
- in automobile polishes, ceramic glazes, laundry starch, inks, and dyes
- in odour agents.

Chemicals in this group have one or more of the following reported commercial uses:

- in metal working fluids, such as cutting emulsions
- in adhesives and binding agents
- in absorbents and adsorbents
- in construction materials
- in impregnation materials
- in leather, textile and wood treatment, rubber, and paper manufacturing.

Chemicals in this group have the following reported site limited uses:

- as an accelerator during dyeing of synthetic fibres
- in manufacturing dyes and thermoplastics (plasticiser)
- in manufacturing polymers, resins, and rubber.

In most cases the functional use of 2-phenylphenol and its salts is as a biocide, preservative, disinfectant, sanitising agent or intermediate in various industries. Chemicals in this group also have reported non-industrial uses in pesticides, therapeutic goods, and food additives in some jurisdictions (NCBIa; NCBIb). These non-industrial uses are outside the scope of this evaluation.

Existing Australian regulatory controls

Obligations apply to report additional information about hazards under *Section 100* and to provide any information specifically required by the terms of the Inventory listing under *Section 101, of the Industrial Chemicals Act 2019.*

Environment

The industrial uses of chemicals in this evaluation are not subject to any specific national environmental regulation.

2-Phenylphenol appears as “ortho-phenylphenol” on the Australian Pesticides and Veterinary Medicine Authority (APVMA) Reserved Chemical Products list. 2PP may be used in agricultural and veterinary products as a disinfectant without requiring product registration .

International regulatory status

United Nations

Chemicals in this evaluation are not currently identified as persistent organic pollutants (UNEP 2001), ozone depleting substances (UNEP 1987), or hazardous substances for the purpose of international trade (UNEP and FAO 1998).

Canada

Environment and Climate Change Canada and Health Canada recently published a draft screening assessment of the sodium salt (using 2-phenylphenol as an analogue), finding that there is a low risk of harm to the environment (Government of Canada 2020).

European Union

The chemical 2PP is permitted to be used as a preservative in cosmetics in the EU at up to 0.2% or 0.15% as phenol in rinse-off products and leave-on products, respectively (SCCS 2015; 2018). S2PP and P2PP are not permitted as cosmetic preservatives.

2-Phenylphenol is approved for use as a biocidal active substance under Biocidal Products Regulation (ECHAa). Biocidal products must be authorised before they can be made available on the market or used in the European Economic Area (EEA) and Switzerland. The regulation authorises the manufacture and use of biocidal and preservative chemicals on the

European market, with the aim of high level consumer and environmental protection. The following product types (PT) are approved (A) or have an initial application (IA) for approval in progress for 2PP (ECHAb):

- PT01 – Human hygiene (A)
- PT02 – Disinfectants and algaecides not intended for direct application to humans or animals (A)
- PT03 – Veterinary hygiene (A)
- PT04 – Food and feed area (A)
- PT06 – Preservatives for products during storage (A)
- PT07 – Film preservatives (IA)
- PT09 – Fibre, leather, rubber, and polymerised materials preservatives (IA)
- PT10 – Construction material preservatives (IA)
- PT13 – Working or cutting fluid preservatives (A).

United States of America

The US EPA recently released an Endocrine Disruptor Screening Program (EDSP) Tier 1 review of 2PP and a draft human health and ecological risk assessment (US EPA 2015; 2019). The EDSP review concluded that there was evidence of potential interaction with the estrogen pathway in fish. Future EDSP Tier 2 testing of 2PP was recommended to better understand potential reproductive effects (US EPA 2015).

Environmental exposure

2-Phenylphenol is a high production volume chemical with a complex variety of industrial and other uses. The primary function of 2-phenylphenol and its salts is as a biocide or preservative in a variety of industrial applications and products ranging from cosmetics to household products, as well as a variety of commercial and site limited uses. It may also have non-industrial use in pesticides and therapeutic goods, but these uses are outside the scope of this evaluation.

The use of chemicals in this evaluation in cosmetic and other consumer use products are expected to result in their release to sewers in wastewater following use. Depending on degradation and partitioning processes of chemicals in sewage treatment plants (STPs), some fraction of the quantity of chemicals in wastewater entering STPs can be emitted to the air compartment, to rivers or oceans and sediment in treated effluent, or to soil by application of biosolids to agricultural land (Struijs 1996). The emissions of 2-phenylphenol and its salts to environmental surface waters, sediment, soil, and air are considered as part of this evaluation.

2-Phenylphenol and its salts are used in a variety of industries and products that may result in release to the environment (sewer, surface waters, air, or soil) through various waste streams. Other uses of the chemical are expected to result in its direct release to the environment.

Environmental monitoring data exists for 2-phenylphenol and is discussed further in the predicted environmental concentration (PEC) section of this Evaluation Statement.

Environmental fate

Dissolution, speciation, and partitioning

Chemicals in this group are expected to partition to the water, soil, and sediment compartments after release to the environment from their industrial use.

As a weak acid, 2-phenylphenol is in pH dependent equilibrium, dissociating to its conjugate base and hydrogen ions. However, in the environmentally relevant pH range, the dominant form is the undissociated free acid. In aqueous environments the very soluble sodium and potassium salts will dissociate into the conjugate base and sodium and potassium ions. At environmentally relevant pH, the free acid will rapidly be formed from the conjugate base, so this will partition in the same way as 2-phenylphenol.

2-Phenylphenol is the environmentally relevant species, and it is classified as moderately volatile (vapour pressure 0.01–1 Pa) and moderately soluble in water (10–1000 mg/L). Its estimated Henry's Law constant (>0.025 $Pa \cdot m^3/mol$) indicates a moderate volatility from water and moist soil (Mensink et al. 1995). The measured log K_{OW} value of 3.18 indicates it is moderately lipophilic and is expected to adsorb more readily to organic matter in soils or sediments due to its lower affinity for water. The measured K_{OC} values ranged between 252–393 L/kg (log K_{OC} 2.4–2.6) (REACHb). This indicates medium mobility in soil (McCall et al. 1980).

Calculations were undertaken with a standard multimedia partitioning (fugacity) model assuming sole emissions to air, water, or soil compartments (Level III approach). If solely emitted to air, 2-phenylphenol will partition predominantly to soil (58%), followed by water (8%) and sediment (2%), with 34% remaining in the air compartment. If emitted solely to water, 2-phenylphenol mostly remains in water (98.4%), with the remainder (1.6%) partitioning to sediment. Emissions to soil will remain in soil (>99%). Fugacity modelling assuming equal emissions to air, water and soil (Level III approach) indicates partitioning to soil (73.6%), water (25.2%), air (0.8%), and sediment (0.4%) (US EPA 2017).

Degradation

2-Phenylphenol is degraded in the environment by natural processes. It is readily biodegradable and undergoes rapid abiotic degradation in both air and water.

In a study conducted according to OECD Testing Guideline (TG) 301B, 2-phenylphenol was found to be readily biodegradable in water based on 70.8–75.7% CO_2 evolution in 28 days. This study measured 62.8–67.7% CO_2 evolution at day 11 and 33.5–65.2% CO_2 evolution at day 3, so the substance is considered very close to or meeting the 10 day ready biodegradation criterion. The study was carried out using low test concentrations of 0.2 mg/L and 1.0 mg/L (REACHb).

The rapid biodegradation of 2PP is supported by the results of three other biodegradation studies in water. In a test conducted according to OECD TG 301E, but using Rhine River water instead of deionised water, 100% biodegradation was reached between 6 and 9 days. In a test following the procedures of the EU method C.4-D, 96% biodegradation was observed after 28 days. An inherent biodegradation study, which was performed according to OECD TG 302 B, showed 100% removal of dissolved organic carbon after 10 days (REACHb). Based on these results ready 10 day biodegradation is assumed.

Persistence in the soil is not expected. A test according to OECD TG 307 showed that the simple first order DT50 value for 2PP in the test soil was 2.7 hours (REACHb).

2-Phenylphenol also undergoes abiotic degradation in air. Phototransformation in air is not particularly relevant due to moderate vapour pressure (<1 Pa at 20 °C). However, calculated values for indirect photodegradation in air indicate degradation is rapid; the half life for reaction with OH-radicals is 0.6 days (24 hour day; OH-concentration: 0.5×10^6 OH/cm^3) (REACHb).

Hydrolysis is not relevant to abiotic degradation in the environment. 2-Phenylphenol does not contain hydrolysable groups and a study according to OECD TG 111 found less than 10% was hydrolysed during 5 days implying a DT50 of more than one year (REACHb).

2-Phenylphenol may undergo phototransformation in environmental waters. 2-Phenylphenol is rapidly photodegraded in water according to two phototransformation studies (DT50 0.3–5.3 days) (REACHb). Photolysis studies conducted with 2PP in air saturated water with irradiation at 296 nm found several photodegradation products. The main three were identified as phenylhydroquinone (PHQ, CAS No. 1079-21-6), phenylbenzoquinone (PBQ, CAS No. 363-03-1), and 2-hydroxydibenzofuran (2OHDBF, CAS No. 86-77-1) (Sarakha et al. 1989; Seffar et al. 1987). Given the rapid biodegradability of 2PP, it is unclear how relevant phototransformation is as a dissipation mechanism in environmental surface waters.

Bioaccumulation

2-Phenylphenol has a low potential to bioaccumulate in aquatic life.

The measured bioconcentration factor (BCF) was found to be 21.7 L/kg whole body wet weight in a study conducted as per EU Method C.13; flow-through fish test on zebra fish, *Danio rerio* (REACHb). Based on the steady-state BCF of 21.7 L/kg, and a log K_{OW} less than 4.2 a significant potential to bioaccumulate is not expected for 2-phenylphenol. The BCF is well below the domestic threshold of 2000 L/kg for aquatic bioaccumulation.

Given log K_{OW} is greater than 2 and the calculated log K_{OA} is greater than 6 (US EPA 2017), bioaccumulation in air breathing animals could be considered, if the chemical is non-metabolising (DAWE 2016; EPHC 2009). However, environmental exposure to air breathing animals is not highly relevant based on use patterns and environmental fate considerations, and the substance is metabolised as demonstrated in animal toxicity studies. However, it is worth noting that 2PP metabolises into other biologically active compounds, including phenylhydroquinone (PHQ) and phenylbenzoquinone (PBQ). Toxicity studies indicate that these are also conjugated and excreted, as the entire administered does is accounted for (Bartels et al. 1998; Bomhard et al. 2002; INCHEM 1999; Köse and Kocasari 2020; Kwok and Silva 2013).

Environmental transport

Chemicals in this group are not expected to undergo long range transport based on their short half lives in the environment.

Predicted environmental concentration (PEC)

The predicted environmental concentration (PEC) of 2PP in surface waters is 0.092 µg/L based on a domestic environmental monitoring study (Scott et al. 2014). A sediment PEC of 0.00145 mg/kg dw was calculated based on the surface water concentration observed by

Scott et al. (2014) using the equilibrium partitioning method (EPHC 2009). The soil PEC was calculated to be 0.43 mg/kg dw based on calculated biosolids concentrations from standard modelling (Struijs 1996).

Standard exposure modelling for the release of chemicals to surface waters from sewage treatment plants (STPs) was used to estimate the concentration of 2PP in river water receiving treated effluents (EPHC 2009; Struijs 1996). Chemicals in this evaluation have several industrial and non-industrial uses, but the relative proportions of each use in Australia are unknown. Therefore, a worst case assumption is made that 100% of the quantity of each chemical introduced for industrial use is released to STPs nationwide. Based on this standard approach and using the cumulative assumed annual introduction volume of 400 tonnes total for 2PP and each of its salts, 88% of the chemical in wastewater entering an STP is predicted to be removed by biodegradation (85%) and partitioning to sludge (3%). The resulting concentration in STP effluent is calculated to be 25.58 µg/L, and 0.43 mg/kg in biosolids.

This calculated concentration is likely to be a significant overestimate of the maximum environmental concentration of 2PP in Australian rivers. A national survey of trace organic contaminants at 73 river sites in mainland Australia found a maximum measured concentration of 0.092 µg/L over a year of monitoring (Scott et al. 2014). Therefore, this value is adopted as the upper limit of surface water concentrations of 2PP in Australia for the purpose of risk characterisation.

This value is consistent with other international and domestic environmental and STP monitoring data for 2PP. A maximum effluent concentration of 0.024 µg/L was measured in a survey of 39 STPs in Victoria, Australia (Allinson et al. 2012). Monitoring at a German sewage treatment plant (STP) with tertiary treatment found that more than 99% of 2PP was eliminated during treatment, resulting in an effluent concentration of less than 0.015 µg/L (Körner et al. 2000).

The calculated 2PP concentration in soil amended with biosolids is 0.43 mg/kg dry weight based on the concentration in biosolids calculated by the SimpleTreat model (version 3.0) (Struijs et al. 1996), typical biosolids application rates and a soil bulk density of 1500 kilograms per cubic metre (kg/m^3) (EPHC 2009).

Environmental effects

2-Phenylphenol exhibits acute and significant chronic toxicity, and there is evidence to suggest it may cause some endocrine mediated effects in fish.

Effects on Aquatic Life

Acute toxicity

The following measured median effective concentration (EC50) and median lethal concentration (LC50) values for freshwater model organisms across three trophic levels were taken from the REACH Registration Dossier for 2-phenylphenol (REACHb):

Taxon	Endpoint	Method
Fish	96 h LC50 = 4.5 mg/L	*Danio rerio* (zebra fish) OECD TG 203 Mortality Semi-static
Invertebrates	48 h EC50 = 2.7 mg/L	*Daphnia magna* (water flea) ASTM Standard E729-80 Mobility Static
Algae	72 h ErC50 = 3.57 mg/L 72 h EC50 = 1.35 mg/L	*Pseudokirchneriella subcapitata* (green algae) OECD TG 201 Growth rate and Biomass Static

Chronic toxicity

The following measured no observed effect concentration (NOEC) values were retrieved from the REACH Registration Dossier for 2-phenylphenol (REACHb) and the summary of the fish reproduction assay in the US EPA review (US EPA 2015):

Taxon	Endpoint	Method
Fish	21 d NOEC = 0.004 mg/L	*Pimephales promelas* (fathead minnow) As per method of Harries et al. (2000) Egg production Flow-through
Invertebrates	21 d NOEC = 0.009 mg/L	*Daphnia magna* (water flea) OECD TG 211 Reproduction Semi-static
Algae	96 h NOEC = 0.432 mg/L	*Pseudokirchneriella subcapitata* (green algae) OECD TG 201 Growth rate Static

Effects on terrestrial Life

2-phenylphenol and salts are not expected to cause toxic effects to terrestrial organisms at low concentrations. Animal toxicity studies have been discussed in detail in previous human health risk assessments of these chemicals (NICNAS 2006; 2015).

The below data have all been retrieved from the REACH dossier for 2-phenylphenol (REACHb).

Ecotoxicity testing on soil macro-organisms in standard soil with 10% added organic matter (sphagnum peat) according to OECD TG 207 found the following:

- 14 d mortality LC50 = 198.2 mg/kg soil dw, *Eisenia fetida* (earthworms)
- 14 d mortality and weight NOEC = 125 mg/kg soil dw, *Eisenia fetida* (earthworms).

Ecotoxicity testing on soil micro-organisms a loamy soil enriched with lucerne meal (concentration in soil 0.5%) according to OECD TG 216 found the following:

- 28 d nitrogen transformation EC50 = 633.5 mg/kg soil dw
- 28 d nitrogen transformation NOEC = 300 mg/kg soil dw.

Ecotoxicity testing on terrestrial plants in sandy loam soil (0.99% organic carbon) according to OECD TG 208 found the following:

- 14 d growth EC50 = 53.9 mg/kg soil dw, *Avena sativa* (common oat)
- 14 d growth NOEC = 12.5 mg/kg soil dw, *Avena sativa* (common oat).

Ecotoxicity testing on birds according to US EPA TG 71-1 found the following:

- 14 d all endpoints NOEC = 2250 mg/kg bw, *Anas platyrhynchos* (mallard duck).

Effects on sediment dwelling life

A test, investigating effects of 2-phenylphenol on larvae of sediment dwelling organisms (*Chironomus riparius*, midges) according to OECD TG 219 is available. A 28-day NOEC value of 1.85 mg/L (spiked water) for the emergence rate was observed (REACHb). Conversion of this NOEC to sediment concentration using the equilibrium partitioning method, and assuming a consistent overlying water concentration of 1.85 mg/L, gives a sediment NOEC of 29.1 mg/kg dw.

Effects on aquatic micro-organisms

A test, investigating effects of 2-phenylphenol on aquatic micro-organisms (domestic sludge) according to OECD T G 209 is available. A 3 h EC50 value of 56 mg/L for respiration rate was observed (REACHb).

Endocrine effects/activity

There is evidence of in vitro and in vivo endocrine activity of 2-phenylphenol. It is listed by The Endocrine Disruption Exchange as a potential endocrine disrupting chemical (TEDX). Endocrine activity screening assays gave positive results in 6 estrogen receptor (ER) assays (out of 20) and 3 androgen receptor (AR) assays (out of 17) (US EPAb). 2PP was found to induce vitellogenin gene expression in rainbow trout hepatocyte cell cultures, though at much lower potency than natural 17β-estradiol (EC 2002).

A Tier 1 EDSP weight of evidence review on the endocrine effects of 2PP was conducted by the US EPA in 2015. This review considered estrogenic, androgenic, and thyroid pathways for mammalian and non-mammalian species, concluding that there is evidence of potential interaction with the estrogen pathway in fish and other non-mammalian species. While a similarly detailed review of the available literature is out of scope for this evaluation, some of the more relevant studies are summarised below.

Some effects on reproductive endpoints in fathead minnow in two 21 day short term reproductive studies using 2PP as the test substance were reported (US EPA 2015). In one test, decreases in vitellogenin levels and a non-significant decrease in fecundity levels were observed at the highest test concentration of 876 µg/L, with no effects observed at the next lowest test concentration of 75.5 µg/L. In the second test, 66% and 94% decreases in egg

production were observed at 2PP concentrations of 36 and 293 µg/L respectively. However, it was noted that there was quite high variability in the egg production numbers in the control group. There were no effects on gonadal somatic index or gonadal histopathology. These in vivo effects, along with indications of potential in vitro effects including ER activation and altered steroidogenesis, suggest that 2PP may potentially interact with the estrogen pathway in fish.

The effect on vitellogenin levels suggests that the substance interacts with the endocrine system in fish, but this effect was only observed at the highest test substance concentration. In addition, the studies show some reproductive effects of 2PP on fathead minnow. However, there is currently inadequate evidence to definitively show that the reproductive effects are endocrine mediated. The US EPA review recommended that a medaka extended one generation reproduction test be conducted to better characterise the reproductive and endocrine mediated effects of this substance in fish (US EPA 2015). It is not known if this test has been conducted.

Predicted no-effect concentration (PNEC)

The freshwater riverine PNEC for 2PP of 0.0004 mg/L (0.4 µg/L) was derived from the chronic fish endpoint (21 d reproduction NOEC = 0.004 mg/L) for this chemical. An assessment factor of 10 was applied to the lowest aquatic NOEC, as reliable chronic ecotoxicity data are available for this chemical from three species representing three trophic levels in water (EPHC 2009).

The soil PNEC of 1.25 mg/kg was derived from the terrestrial plants' endpoint (14 d growth NOEC of 12.5 mg/kg soil dw for common oat) for this chemical. An assessment factor of 10 was applied to the lowest soil NOEC, as reliable chronic ecotoxicity data are available for this chemical from three species representing three trophic levels in soil (EPHC 2009). This value was derived without any normalisation for soil organic carbon content.

The sediment PNEC of 0.291 mg/kg dw was derived from the measured *Chironomus riparius* 28-day NOEC of 1.85 mg/L (converted to 29.1 mg/kg dw using the equilibrium partitioning method). An assessment factor of 100 was applied, as reliable chronic ecotoxicity data are available for one taxon (EPHC 2009).

Categorisation of environmental hazard

The categorisation of the environmental hazards of the assessed chemicals according to domestic environmental hazard thresholds is presented below:

Persistence

Not Persistent (Not P). Based on measured ready biodegradability and rapid abiotic degradation, 2-phenylphenol and its salts are categorised as Not Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on low measured bioconcentration factors (BCF) in fish and a log K_{OW} value less than 4.2, and evidence of biotransformation, 2-phenylphenol and its salts are categorised as Not Bioaccumulative.

Toxicity

Toxic (T). Based on evidence of high chronic toxicity for rapidly degradable substances (ecotoxicity values below 0.01 mg/L), 2-phenylphenol and its salts are categorised as Toxic.

Environmental risk characterisation

Based on the PEC and PNEC values determined above, the following Risk Quotients (RQ = PEC ÷ PNEC) have been calculated for release into rivers, soil, and sediment:

Compartment	PEC	PNEC	RQ
Riverine	0.092 µg/L	0.4 µg/L	0.23
Soil	0.43 mg/kg	1.25 mg/kg	0.34
Sediment	0.00145 mg/kg	0.291mg/kg	0.005

The RQs less than 1 indicate that 2-phenylphenol is not expected to pose an unreasonable risk to the environment from release to water, soil and sediment in Australia based on the estimated emissions, as environmental concentrations are below the levels likely to cause harmful effects.

There is evidence to suggest that chemicals in this evaluation may have potential to cause endocrine mediated effects. However, the contribution to the overall hazard characteristics of the chemical in Australia is uncertain. The aquatic PNEC has been calculated from the lowest chronic ecotoxicity endpoint for fish, which is expected to account for the possibility of endocrine mediated effects based on currently available evidence.

Uncertainty

This evaluation was conducted based on information that may be incomplete or limited in scope. Some relatively common data limitations can be addressed through use of conservative assumptions (OECD 2019) or quantitative adjustments such as assessment factors (OECD 1995). Others must be addressed qualitatively, or on a case by case basis (OECD 2019).

The most consequential areas of uncertainty for this evaluation are:

- There are no domestic monitoring data for 2-phenylphenol in sediment or soil compartments. The risk profile for these chemicals may change should monitoring data become available to indicate that these chemicals are present in Australian sediments and soils at concentrations above the level of concern.
- There is no domestic use volume data available for 2-phenylphenol and the sodium salts. The risk profile of 2-phenylphenol and salts may change should use volume or monitoring data become available to indicate that these chemicals are present in Australian surface waters, sediments, or soils at levels above the levels of concern.
- The environmental properties and effects of degradants and metabolites of 2-phenylphenol (including phenylbenzoquinone, phenylhydroquinone and 2-hydroxydibenzofuran) are largely unknown. The risk profile of 2-phenylphenol and salts may change if information becomes available to indicate that these degradants and metabolites are more hazardous than the parent chemical.
- The potential for 2-phenylphenol to cause endocrine mediated effects has not been completely characterised. Weight of evidence reviews based on literature and studies available at the time demonstrated potential endocrine mediated effects for fish, with

some uncertainties still apparent and further studies recommended. The risk profile of 2-phenylphenol and salts may change if additional information about the endocrine effects of these chemicals becomes available.

References

Allinson M, Kageyama S, Nakajima D, Kamata R, Shiraishi F, Goto S, Salzman S and Allinson G (2012). A pilot survey of 39 Victorian WWTP effluents using a high speed luminescent umu test in conjunction with a novel GC-MS-database technique for automatic identification of micropollutants. *Water science and technology: a journal of the International Association on Water Pollution Research,* 66(4):768-774, doi:10.2166/wst.2012.242.

APVMA (Australian Pesticides and Veterinary Medicines Authority) (2021) *Reserved Chemical Products*, APVMA, accessed December 2021.

Bartels MJ, McNett DA, Timchalk C, Mendrala AL, Christenson WR, Sangha GK, Brzak KA and Shabrang SN (1998). Comparative metabolism of ortho-phenylphenol in mouse, rat and man. *Xenobiotica; the fate of foreign compounds in biological systems,* 28(6): 579-594, doi: 10.1080/004982598239335.

Bomhard EM, Brendler-Schwaab SY, Freyberger A, Herbold BA, Leser KH and Richter M (2002). O-Phenylphenol and its Sodium and Potassium Salts: A Toxicological Assessment. *Critical Reviews in Toxicology,* 32(6):551-626, doi:10.1080/20024091064318.

CEPA (California Environment Protection Agency) (2007) *Ortho-Phenylphenol (OPP) and Sodium Ortho-Phenylphenate (SOPP) Risk Characterization Document Dietary Exposures*. CEPA, accessed December 2021.

CEPA (California Environment Protection Agency) (2016) *Completion of mitigation for dietary exposure to ortho-phenylphenol and its sodium and potassium salts*. CEPA, accessed December 2021.

Chemwatch (n.d.) *Data for o-phenylphenol (CAS No. 90-43-7)*, Galleria Chemica, Chemwatch website, accessed December 2021.

DAWE (Department of Agriculture, Water and the Environment) (2016). *Draft National Standard for Environmental Risk Management of Industrial Chemicals Explanatory Document*, DAWE, accessed December 2021.

ECCC (Environment and Climate Change Canada) (n.d.) *Categorization Results from the Canadian Domestic Substance List (CAS No. 90-43-7)*, ECCC website, accessed December 2021.

ECHAa (European Chemicals Agency) (n.d.) *Information on biocides - biocidal active substances - biphenyl-2-ol*, ECHA website, accessed December 2021.

ECHAb (European Chemicals Agency) (n.d.) *Biocidal Products Directive: Information on Biocides*, ECHA website, accessed December 2021.

EPHC (Environment Protection and Heritage Council) (2009) *Environmental Risk Assessment Guidance Manual for Industrial Chemicals*, EPHC, accessed December 2021.

EC (European Commission) (2002) *Study on the scientific evaluation of 12 substances in the context of endocrine disruptor priority list of actions - O-phenylphenol*. EC, accessed December 2021.

EC (European Commission) (n.d.) *Database for information on cosmetic substances and ingredients (CosIng): o-phenylphenol*, EC website, accessed December 2021.

Fiege H, Voges H-W, Hamamoto T, Umemura S, Iwata T, Miki H, Fujita Y, Buysch H-J, Garbe D and Paulus W (2012) Phenol Derivatives. In: Interscience W, ed. *Ullmann's Encyclopedia of Industrial Chemistry*. Wiley-VCH GmbH & Co, Weinheim, Germany.

German Research Foundation (Deutsche Forschungsgemeinschaft) (2020). *List of MAK and BAT Values 2020: Maximum Concentrations and Biological Tolerance Values at the Workplace*. Deutsche Forschungsgemeinschaft, accessed December 2021.

Government of Canada (2020) *Draft Screening Assessment: [1,1'-Biphenyl]-2-ol, sodium salt (Sodium ortho-phenylphenate; SOPP)*. Government of Canada, accessed Deember 2021.

Harries JE, Runnalls T, Hill E, Harris CA, Maddix S, Sumpter JP and Tyler CR (2000). Development of a Reproductive Performance Test for Endocrine Disrupting Chemicals Using Pair-Breeding Fathead Minnows (Pimephales promelas). *Environmental Science & Technology,* 34(14): 3003-3011, doi:10.1021/es991292a.

Haz-Map (n.d.) *Haz-Map Hazardous Agents: o-Phenylphenol*, Haz-Map website, accessed December 2021.

IARC (International Agency for Research on Cancer) (1999) IARC Monographs on the Evaluation of Carcinogenic Risks to Humans Volume 73: Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances, *Ortho-phenylphenol and its sodium salt MON73-21*. IARC, accessed December 2021.

INCHEM (Chemical Safety Information from Intergovernmental Organizations) (1999) *Toxicological evaluations: 2-Phenylphenol and its sodium salt*, International Programme on Chemical Safety (IPCS) INCHEM, accessed December 2021.

Körner W, Bolz U, Süßmuth W, Hiller G, Schuller W, Hanf V and Hagenmaier H (2000). Input/output balance of estrogenic active compounds in a major municipal sewage plant in Germany. *Chemosphere,* 40(9):1131-1142, doi:10.1016/S0045-6535(99)00362-8.

Köse SE and Kocasari F (2020). Toxicity of Ortho-Phenylphenol (OPP) and Sodium Ortho-Phenylphenate (SOPP). *Mehmet Akif Ersoy Üniversitesi Sağlık Bilimleri Enstitüsü Dergisi,* 8(1):18-29, doi:10.24998/maeusabed.701208.

Kwok ESC and Silva MH (2013). Re-evaluation of Developmental and Reproductive Toxicity of Ortho-Phenylphenol (OPP) and Sodium Ortho-Phenylphenate (SOPP). *Cell and Developmental Biology,* 2(123):1-12, doi:10.4172/2168-9296.1000123.

LMC (2021) *The OECD QSAR Toolbox*, (Version 4.4.1), [Computer software], Laboratory of Mathematical Chemistry (LMC), University "Prof. Dr. Assen Zlatarov", accessed December 2021.

McCall PJ, Swann RL, Laskowski DA, Unger SM, Vrona SA and Dishburger HJ (1980). Estimation of chemical mobility in soil from liquid chromatographic retention times. *Bulletin of Environmental Contamination and Toxicology,* 24(1):190-195, doi:10.1007/BF01608096.

Mensink B, Montforts M, Wijkhuizen-Maślankiewicz L, Tibosch H and Linders J (1995) Report No. 679101022, Appendix 5, *Manual for summarising and evaluating the*

environmental aspects of pesticides. National Institute of Public Health and Environmental Protection, accessed December 2021.

NCBIa (National Center for Biotechnology Information) (n.d.) *PubChem Compound Summary for CID 7017, 2-phenylphenol*, National Library of Medicine (US), NCBI website, accessed December 2021.

NCBIb (National Center for Biotechnology Information) (n.d.) *PubChem Annotation Record for o-Phenylphenol, Source: Hazardous Substances Data Bank (HSDB)*, National Library of Medicine (USA), NCBI website, accessed December 2021.

NICNAS (National Industrial Chemicals Notification and Assessment Scheme) (2006) *Full Public Report STD/1192: Component of Preventol OF 45 (Potassium phenylphenol human health and environment assessment)* NICNAS, accessed December 2021.

NICNAS (National Industrial Chemicals Notification and Assessment Scheme) (2015) *IMAP Group Assessment Report: Biphenylol and its sodium salt: Human health tier II assessment*. NICNAS, accessed December 2021.

NITE (National Institute of Technology and Evaluation) (n.d.) *Japan CHEmicals Collaborative Knowledge Database (J-CHECK) (CAS No. 90-43-7)*, NITE website, accessed December 2021.

OECD (Organisation for Economic Co-operation and Development) (1995) *Guidance document for aquatic effects assessment*. OECD, Paris, France.

OECD (Organisation for Economic Co-operation and Development) (2009) Environment, Health and Safety Publications Series on Testing and Assessment No. 112, *The 2007 OECD list of high production volume chemicals - ENV/JM/MONO(2009)40*. OECD website, accessed December 2021.

OECD (Organisation for Economic Co-operation and Development) (2019) *Guiding Principles and Key Elements for Establishing a Weight of Evidence for Chemical Assessment, Series on Testing and Assessment No. 311*, OECD website, accessed December 2021.

OECD (Organisation for Economic Co-operation and Development) (n.d.) *Existing Chemicals Database*, OECD website, accessed December 2021.

REACHa (Registration, Evaluation, Authorisation and Restriction of Chemicals) (n.d.) *Registration dossier for sodium 2-biphenylate (CAS No. 132-27-4)*, European Chemicals Agency website, accessed December 2021.

REACHb (Registration, Evaluation, Authorisation and Restriction of Chemicals) (n.d.) *Registration dossier for biphenyl-2-ol (CAS No. 90-43-7)*, European Chemicals Agency website, accessed December 2021.

Sarakha M, Dauphin G and Boule P (1989). Photochemical behaviour of 2-biphenylol in acidic aqueous solution. *Chemosphere,* 18(7-8):1391-1399, doi:10.1016/0045-6535(89)90030-1.

SCCS (European Commission Scientific Committee on Consumer Safety) (2015) *Opinion on o-Phenylphenol, Sodium o-phenylphenate and Potassium o-phenylphenate, 25 June 2015, SCCS/1555/15, revision of 15 December 2015*. SCCS, accessed December 2021.

SCCS (Scientific Commission on Consumer Safety) (2018) *Addendum to the scientific opinion on the use as preservative of o-Phenylphenol, Sodium o-phenylphenate and Potassium o-phenylphenate- Here: the use as preservative of Sodium o-phenylphenate, Potassium o-phenylphenate, MEA o-Phenylphenate 21-22/02/2018, SCCS/1597/18*. SCCS, accessed December 2021.

Scott PD, Bartkow M, Blockwell SJ, Coleman HM, Khan SJ, Lim R, McDonald JA, Nice H, Nugegoda D, Pettigrove V, Tremblay LA, Warne MSJ and Leusch FDL (2014). A national survey of trace organic contaminants in Australian rivers. *Journal of Environmental Quality,* 43:1702-1712, doi:10.2134/jeq2014.01.0012.

Seffar A, Dauphin G and Boule P (1987). Oxidative photocyclisation of 2-biphenylol in dilute aqueous solution. *Chemosphere,* 16(6):1205-1214, doi:10.1016/0045-6535(87)90057-9.

SPIN (Substances in Preparations in Nordic Countries) (n.d.) *SPIN Database*, SPIN website, accessed December 2021.

Struijs J (1996) *SimpleTreat 3.0: a model to predict the distribution and elimination of chemicals by sewage treatment plants*. National Institute of Public Health and the Environment, Bilthoven, The Netherlands.

TEDX (The Endocrine Disruptors Exchange) (n.d.) *List of Potential Endocrine Disruptors*, TEDX website, accessed December 2021.

UNECE (United Nations Economic Commission for Europe) (2017) *Globally Harmonized System of Classification and Labelling of Chemicals (GHS), Seventh Revised Edition*, UNECE, accessed December 2021.

UNEP (United Nations Environment Programme) (1987) *The Montreal Protocol on Substances that Deplete the Ozone Layer*, UNEP, accessed December 2021.

UNEP (United Nations Environment Programme) (2001) *The Stockholm Convention on Persistent Organic Pollutants*, UNEP, accessed December 2021.

UNEP and FAO (United Nations Environment Programme and Food and Agriculture Organization) (1998) *Rotterdam Convention on the Prior Informed Consent Procedure for Certain Hazardous Chemicals and Pesticides in International Trade*, UNEP and FAO, accessed December 2021.

US EPA (United States Environmental Protection Agency) (2015) *EDSP Weight of Evidence Analysis of Potential Interaction with the Estrogen, Androgen or Thyroid Pathways; Chemical: o-phenylphenol*. US EPA, accessed December 2021.

US EPA (United States Environmental Protection Agency) (2017) *Estimation Programs Interface (EPI) Suite™ for Microsoft Windows®, (Version 4.11)*, [Computer software], US EPA, accessed December 2021.

US EPA (United States Environmental Protection Agency) (2019) *Ortho-Phenylphenol and Salts Human Health and Ecological Draft Risk Assessment*. US EPA, accessed December 2021.

US EPAa (United States Environmental Protection Agency) (n.d.) *High Production Volume List*, US EPA website, accessed December 2021.

US EPAb (United States Environmental Protection Agency) (n.d.) *CompTox Chemicals Dashboard, 2-Phenylphenol, DSSTox Substance ID 2021151*, US EPA website, accessed December 2021.

Weber M, Weber M and Kleine-Boymann M (2012) Phenol. In: Interscience W, ed. *Ullmann's Encyclopedia of Industrial Chemistry*. Wiley-VCH Verlag GmbH & Co, Weinheim, Germany.

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