



Australian Government

Department of Health, Disability and Ageing

Australian Industrial Chemicals Introduction Scheme

Alkyl and aryl substituted para-phenylenediamines

Evaluation statement (EVA00207)

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Draft



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AICIS evaluation statement (EVA00207)

Subject of the evaluation

Alkyl and aryl substituted para-phenylenediamines

Chemicals in this evaluation

CAS name	CAS number
1,4-Benzenediamine, <i>N</i> ¹ , <i>N</i> ⁴ -diphenyl-	74-31-7
1,4-Benzenediamine, <i>N,N'</i> -di-2-naphthalenyl-	93-46-9
1,4-Benzenediamine, <i>N</i> -(1-methylethyl)- <i>N'</i> -phenyl-	101-72-4
1,4-Benzenediamine, <i>N</i> -cyclohexyl- <i>N'</i> -phenyl-	101-87-1
1,4-Benzenediamine, <i>N,N'</i> -bis(1-methylpropyl)-	101-96-2
1,4-Benzenediamine, <i>N</i> -(1-methylpropyl)- <i>N'</i> -phenyl-	788-17-0
1,4-Benzenediamine, <i>N</i> ¹ -(1,3-dimethylbutyl)- <i>N</i> ⁴ -phenyl-	793-24-8
1,4-Benzenediamine, <i>N</i> -(1,4-dimethylpentyl)- <i>N'</i> -phenyl-	3081-01-4
1,4-Benzenediamine, <i>N,N'</i> -bis(1,4-dimethylpentyl)-	3081-14-9
1,4-Benzenediamine, <i>N,N'</i> -dicyclohexyl-	4175-38-6
1,4-Benzenediamine, <i>N,N'</i> -bis(1-methylethyl)-	4251-01-8
1,4-Benzenediamine, <i>N,N'</i> -bis(methylphenyl)-	27417-40-9
1,4-benzenediamine, <i>N,N'</i> -mixed phenyl and tolyl and xylyl derivatives	68953-83-3
1,4-Benzenediamine, <i>N,N'</i> -mixed phenyl and tolyl derivatives	68953-84-4

Reason for the evaluation

Evaluation Selection Analysis (ESA) indicated a potential environmental risk

Parameters of evaluation

This evaluation considers the environmental risks associated with the industrial uses of a group of 14 alkyl and aryl substituted *para*-phenylenediamines that are listed on the Australian Inventory of Industrial Chemicals (the Inventory). These chemicals have been assessed as a group because they have similar chemical characteristics, similar uses and their release to the environment is expected to occur in similar ways.

The chemicals in this group have been assessed for their risks to the environment according to the following parameters:

- industrial uses as listed in the 'Summary of introduction, use and end use' section
- expected releases to the soil, air and water compartments as a result of their industrial uses.

In this evaluation, chemical names have been abbreviated according to the type of substituent and/or the number of carbons in the alkyl chain bound to the central *para*-phenylenediamine group. The following abbreviated names, are used throughout this evaluation:

CAS RN	Substituents	Abbreviated name
74-31-7	Phenyl and phenyl	DPPD
93-46-9	Naphthyl and naphthyl	DNPD
101-72-4	Isopropyl and phenyl	IPPD
101-87-1	Cyclohexyl and phenyl	CPPD
101-96-2	Isobutyl and isobutyl	44PD
788-17-0	Isobutyl and phenyl	4PPD
793-24-8	Dimethyl butyl and phenyl	6PPD
3081-01-4	Dimethyl pentyl and phenyl	7PPD
3081-14-9	Dimethyl pentyl and dimethyl pentyl	77PD
4175-38-6	Cyclohexyl and cyclohexyl	CCPD
4251-01-8	Isopropyl and isopropyl	33PD
27417-40-9	Tolyl and tolyl (any isomers)	DTPD
68953-83-3	UVCB with phenyl and phenyl, phenyl and tolyl, phenyl and xylyl, tolyl and xylyl, and xylyl and xylyl	PaTaXPD
68953-84-4	UVCB with phenyl and phenyl, phenyl and tolyl, and tolyl and tolyl	PaTPD

Two of the chemicals have previously been assessed, either under AICIS or under the former National Industrial Chemicals Notification and Assessment Scheme (NICNAS):

- DTPD (CAS RN 27417-40-9); previously published as a chemical unlikely to be commercially active in Australia (AICIS 2022a), and
- PaTaXPD (CAS RN 68953-83-3); previously assessed under NICNAS (NICNAS 2001).

These chemicals have been included in the evaluation to provide information on the environmental hazards or exposure to these chemicals.

Another related chemical is discussed throughout the evaluation:

- 8PPD; methylheptyl and phenyl substituted *para*-phenylenediamines (CAS RN 15233-47-3).

This chemical has been previously assessed under the former NICNAS but has not been included in this evaluation because no new information has become available to suggest that re-evaluation is required.

Summary of evaluation

Summary of introduction, use and end use

Chemicals in this evaluation have functional use as antioxidants or as antiozonants in the following products according to Australian and international use data:

- plastic and polymer products
- fuel, oil, fuel oil additives and related products
- lubricant and grease products.

Australian use volume information is available for one chemical in the group. A volume of 100–1,000 tonnes/year was reported for 6PPD.

Reported volumes from international jurisdictions indicate that six of the chemicals are introduced in volumes >1000 tonnes. 6PPD has the highest reported volume in use globally.

Environment

Summary of environmental hazard characteristics

Based on the information presented in this evaluation and according to the environmental hazard thresholds stated in the Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals (DCCEEW 2022), DNPD (CAS RN 93-46-9), DTPD (CAS RN 27417-40-9), PaTaXPD (CAS RN 68953-83-3) and PaTPD (CAS RN 68953-84-4) are:

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

All other chemicals in this evaluation are:

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

Environmental hazard classification

The chemicals in this evaluation satisfy the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) (UNECE 2017) for environmental hazards. This evaluation does not consider classification of physical or human health hazards.

Classifications were primarily based on available experimental ecotoxicity information and degradability information. Some of the proposed hazard classifications are based on read across principles (see **Supporting information**).

The following chemicals are classified according to the table below:

- DPPD (CAS RN 74-31-7)
- DNPD (CAS RN 93-46-9)
- 6PPD (CAS RN 793-24-8)
- DTPD (CAS RN 27417-40-9)
- PaTaXPD (CAS RN 68953-83-3)
- PaTPD (CAS RN 68953-84-4).

Environmental Hazard	Hazard Category	Hazard Statement
Hazardous to the aquatic environment (acute / short-term)	Aquatic Acute 1	H400: Very toxic to aquatic life
Hazardous to the aquatic environment (long-term)	Aquatic Chronic 1	H410: Very toxic to aquatic life with long lasting effects

The following chemicals are classified according to the table below:

- IPPD (CAS RN 101-72-4)
- 44PD (CAS RN 101-96-2).

Environmental Hazard	Hazard Category	Hazard Statement
Hazardous to the aquatic environment (acute / short-term)	Aquatic Acute 1	H400: Very toxic to aquatic life
Hazardous to the aquatic environment (long-term)	Aquatic Chronic 2	H411: Toxic to aquatic life with long lasting effects

The following chemicals are classified according to the table below:

- CPPD (CAS RN 101-87-1)
- 4PPD (CAS RN 788-17-0)
- 7PPD (CAS RN 3081-01-4)
- 77PD (CAS RN 3081-14-9)
- CCPD (CAS RN 4175-38-6)
- 33PD (CAS RN 4251-01-8).

Environmental Hazard	Hazard Category	Hazard Statement
Hazardous to the aquatic environment (acute / short-term)	Aquatic Acute 1	H400: Very toxic to aquatic life

Summary of environmental risk

Based on available Australian and international use information, chemicals in this evaluation are expected to be used in Australia as additives in rubber and plastic articles, and fuel and lubricant products. The primary release of the chemicals is expected to occur via tyre wear particles, resulting in exposure of roadside soils, waterways receiving road runoff, and sediments to the chemicals and their degradants. Other uses of these chemicals are not expected to result in significant releases to the environment.

The chemicals in this evaluation transform in water, sediment and soil under degradation test conditions and are not persistent. Oxidation and ozonation of the chemicals in water or on surfaces, such as rubber, can result in the formation of substituted *para*-phenylenediamine-quinone degradants.

The chemicals, DNPD and DTPD, exceed thresholds for bioaccumulation in aquatic organisms. PaTPD is a UVCB substance that is known to contain DTPD. Therefore, PaTPD is bioaccumulative. PaTaXPD contains DTPD and other constituents that exceed thresholds for bioaccumulation. Therefore, PaTaXPD is bioaccumulative. The remaining chemicals do not meet thresholds for bioaccumulation based on log K_{OW} values below 4.2 or estimated or experimental bioconcentration factors below 2,000 L/kg.

All chemicals in this evaluation are toxic to aquatic organisms. The degradant of 6-PPD, 6PPD-quinone (6PPD-q; CAS RN 2754428-18-5) is especially toxic to salmonid fish species.

Based on the available monitoring data for Australian surface waters and international monitoring data for water and sediments, the concentrations of the chemicals in this evaluation, and the degradants resulting from their use, are expected to be below levels of concern.

The calculated risk quotients (RQs) for the chemicals in this evaluation in surface waters are less than 1. Limited data are available to assess the risks of all chemicals in this evaluation to sediment dwelling life. The calculated RQ for 6PPD in sediments is less than 1. The calculated RQs for 6PPD-q in surface waters and sediments are less than 1. Available information indicates that the risks to aquatic life from other PPD-quinones are lower than the risk from 6PPD-q. Therefore, the current industrial use of these chemicals in Australia is not expected to pose a significant risk to the environment.

Conclusions

The Executive Director is satisfied that the identified risks to human health and the environment from the introduction and use of the industrial chemical can be managed.

Note:

1. Obligations to report additional information about hazards under section 100 of the *Industrial Chemicals Act 2019* apply.
2. You should be aware of your obligations under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory.

Supporting information

Grouping rationale

This evaluation considers the environmental risks associated with the industrial uses of a group of 14 alkyl and aryl substituted *para*-phenylenediamines (PPDs). Chemicals in this evaluation are used in high volumes worldwide and were selected for evaluation because the evaluation selection analysis (ESA) indicated a potential risk to the environment. These chemicals have been assessed as a group as they have similar chemical structures, industrial uses and environmental release patterns.

Two chemicals previously assessed under NICNAS or AICIS were included in this evaluation. They were included in the evaluation group to provide information on the hazards or exposure of the chemicals.

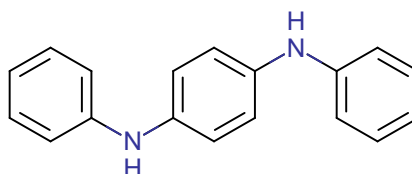
Another related chemical previously assessed under NICNAS was identified. However no new information has become available to suggest re-evaluation of the chemical is required.

Chemical identity

The substances in this evaluation are members of a large group of compounds known as substituted *para*-phenylenediamines. They all have a core structure comprising a benzene ring with amine groups at the 1- and 4-carbon positions (*para*). Each amine group is substituted with either alkyl or aryl moieties. The chemicals in this evaluation differ in the combinations of alkyl and/or aryl substituents attached to the amine groups.

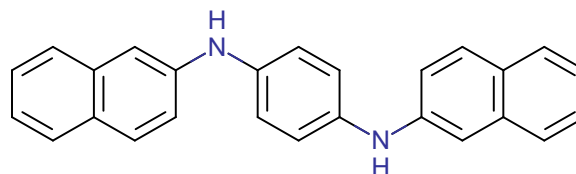
CAS number	74-31-7
CAS name	1,4-Benzenediamine, <i>N</i> ¹ , <i>N</i> ⁴ -diphenyl-
Molecular formula	C ₁₈ H ₁₆ N ₂
Associated names	DPPD 1,4-Benzenediamine, <i>N,N'</i> -diphenyl- <i>p</i> -Phenylenediamine, <i>N,N'</i> -diphenyl-
Molecular weight (g/mol)	260.33
SMILES (canonical)	<chem>C=1C=CC(=CC1)NC2=CC=C(C=C2)NC=3C=CC=C3</chem>

Structural formula

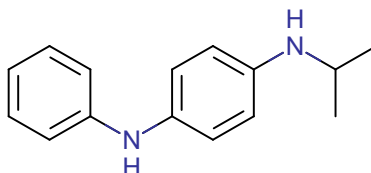


CAS number	93-46-9
CAS name	1,4-Benzenediamine, <i>N,N'</i> -di-2-naphthalenyl-
Molecular formula	C ₂₆ H ₂₀ N ₂
Associated names	DNPD 1- <i>N</i> ,4- <i>N</i> -Dinaphthalen-2-ylbenzene-1,4-diamine <i>N,N'</i> -Di-2-naphthyl- <i>p</i> -phenylenediamine
Molecular weight (g/mol)	360.45
SMILES (canonical)	<chem>C=1C=CC=2C=C(C=CC2C1)NC3=CC=C(C=C3)NC=4C=CC=5C=CC=CC5C4</chem>

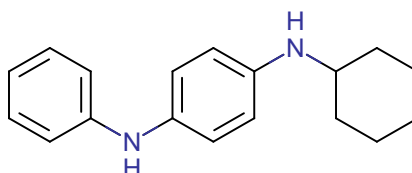
Structural formula



CAS number	101-72-4
CAS name	1,4-Benzenediamine, <i>N</i> -(1-methylethyl)- <i>N'</i> -phenyl-
Molecular formula	C ₁₅ H ₁₈ N ₂
Associated names	IPPD 1- <i>N</i> -Phenyl-4- <i>N</i> -propan-2-ylbenzene-1,4-diamine <i>N</i> -Isopropyl- <i>N'</i> -phenyl- <i>p</i> -phenylenediamine <i>N</i> -Isopropyl- <i>N'</i> -phenyl-1,4-phenylenediamine 4-Isopropylaminodiphenylamine 226.32
SMILES (canonical)	C=1C=CC(=CC1)NC2=CC=C(C=C2)NC(C)C
Structural formula	



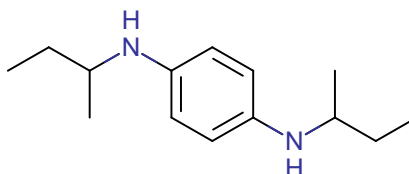
CAS number	101-87-1
CAS name	1,4-Benzenediamine, <i>N</i> -cyclohexyl- <i>N'</i> -phenyl-
Molecular formula	C ₁₈ H ₂₂ N ₂
Associated names	1- <i>N</i> -Cyclohexyl-4- <i>N</i> -phenylbenzene-1,4-diamine <i>N'</i> -Cyclohexyl- <i>N'</i> -phenylbenzene-1,4-diamine <i>N</i> -Cyclohexyl- <i>N'</i> -phenyl- <i>p</i> -phenylenediamine 266.38
SMILES (canonical)	C=1C=CC(=CC1)NC2=CC=C(C=C2)NC3CCCCC3
Structural formula	



CAS number 101-96-2
CAS name 1,4-Benzenediamine, *N,N'*-bis(1-methylpropyl)-
Molecular formula C₁₄H₂₄N₂
Associated names 44PD

p-Phenylenediamine, *N,N'*-di-sec-butyl-
1-*N*,4-*N*-Di(butan-2-yl)benzene-1,4-diamine
N,N'-Di-sec-butyl-*p*-phenylenediamine

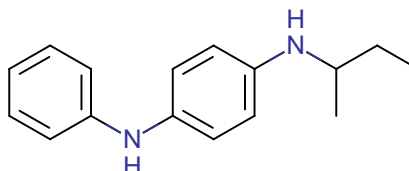
Molecular weight (g/mol) 220.35
SMILES (canonical) C=1C=C(C=CC1NC(C)CC)NC(C)CC
Structural formula



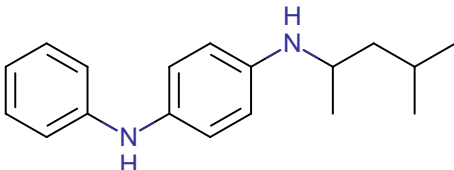
CAS number 788-17-0
CAS name 1,4-Benzenediamine, *N*-(1-methylpropyl)-*N'*-phenyl-
Molecular formula C₁₆H₂₀N₂
Associated names 4-*N*-Butan-2-yl-1-*N*-phenylbenzene-1,4-diamine

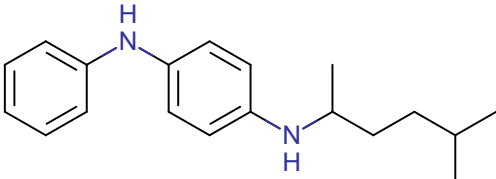
N-(1-Methylpropyl)-*N'*-phenylbenzene-1,4-diamine
p-Phenylenediamine, *N*-sec-butyl-*N'*-phenyl-

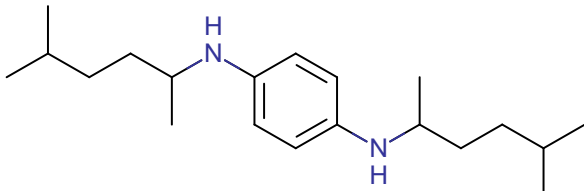
Molecular weight (g/mol) 240.34
SMILES (canonical) C=1C=CC(=CC1)NC2=CC=C(C=C2)NC(C)CC
Structural formula

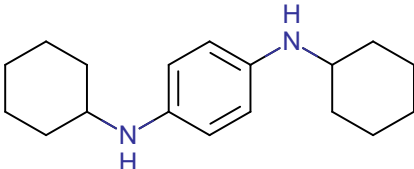


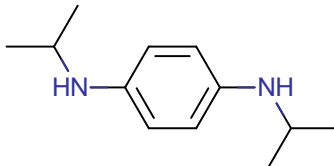
CAS number 793-24-8

CAS name	1,4-Benzenediamine, <i>N</i> ¹ -(1,3-dimethylbutyl)- <i>N</i> ⁴ -phenyl-
Molecular formula	C ₁₈ H ₂₄ N ₂
Associated names	6PPD <i>N</i> ¹ -(1,3-Dimethylbutyl)- <i>N</i> ⁴ -phenyl-1,4-benzenediamine <i>p</i> -Phenylenediamine, <i>N</i> -(1,3-dimethylbutyl)- <i>N</i> '-phenyl-
Molecular weight (g/mol)	268.40
SMILES (canonical)	C=1C=CC(=CC1)NC2=CC=C(C=C2)NC(C)CC(C)C
Structural formula	

CAS number	3081-01-4
CAS name	1,4-Benzenediamine, <i>N</i> -(1,4-dimethylpentyl)- <i>N</i> '-phenyl-
Molecular formula	C ₁₉ H ₂₆ N ₂
Associated names	7PPD <i>p</i> -Phenylenediamine, <i>N</i> -(1,4-dimethylpentyl)- <i>N</i> '-phenyl- 4- <i>N</i> -(5-Methylhexan-2-yl)-1- <i>N</i> -phenylbenzene-1,4-diamine <i>N</i> -(1,4-Dimethylpentyl)- <i>N</i> '-phenylbenzene-1,4-diamine
Molecular weight (g/mol)	282.42
SMILES (canonical)	C=1C=CC(=CC1)NC2=CC=C(C=C2)NC(C)CCC(C)C
Structural formula	

CAS number	3081-14-9
CAS name	1,4-Benzenediamine, <i>N,N'</i> -bis(1,4-dimethylpentyl)-
Molecular formula	C ₂₀ H ₃₆ N ₂
Associated names	77PD 1- <i>N</i> ,4- <i>N</i> -Bis(5-methylhexan-2-yl)benzene-1,4-diamine 1,4-Benzenediamine, <i>N,N'</i> -bis(1,4-dimethylpentyl)- <i>N,N'</i> -Bis(1,4-dimethylpentyl)-phenylenediamine
Molecular weight (g/mol)	304.51
SMILES (canonical)	<chem>C=1C=C(C=CC1NC(C)CCC(C)C)NC(C)CCC(C)C</chem>
Structural formula	

CAS number	4175-38-6
CAS name	1,4-Benzenediamine, <i>N,N'</i> -dicyclohexyl-
Molecular formula	C ₁₈ H ₂₈ N ₂
Associated names	1- <i>N</i> ,4- <i>N</i> -Dicyclohexylbenzene-1,4-diamine <i>N,N'</i> -Dicyclohexyl-4-phenylenediamine <i>p</i> -Phenylenediamine, <i>N,N'</i> -dicyclohexyl-
Molecular weight (g/mol)	272.43
SMILES (canonical)	<chem>C=1C=C(C=CC1NC2CCCCC2)NC3CCCCC3</chem>
Structural formula	

CAS number	4251-01-8
CAS name	1,4-Benzenediamine, <i>N,N'</i> -bis(1-methylethyl)-
Molecular formula	C ₁₂ H ₂₀ N ₂
Associated names	<i>N,N'</i> -Diisopropyl- <i>p</i> -phenylenediamine 1- <i>N</i> ,4- <i>N</i> -Di(propan-2-yl)benzene-1,4-diamine <i>N,N'</i> -Bis(1-methylethyl)benzene-1,4-diamine 1,4-Benzenediamine, <i>N</i> ¹ , <i>N</i> ⁴ -bis(1-methylethyl)-
Molecular weight (g/mol)	192.30
SMILES (canonical)	C=1C=C(C=CC1NC(C)C)NC(C)C
Structural formula	

CAS number	27417-40-9
CAS name	1,4-Benzenediamine, <i>N,N'</i> -mixed phenyl and tolyl derivatives
Molecular formula	C ₂₀ H ₂₀ N ₂
Associated names	<i>N,N'</i> -ditolyl- <i>p</i> -phenylenediamine DTPD
Molecular weight (g/mol)	288.40
SMILES (canonical)	-

Additional chemical identity information

UVCB - this chemical is expected to contain tolyl and tolyl substituted constituents, with unspecified *ortho*-, *meta*-, or *para*- isomerisation of the tolyl constituents.

CAS number	68953-83-3
CAS name	1,4-benzenediamine, <i>N,N'</i> -mixed phenyl and tolyl and xylyl derivatives
Molecular formula	Unspecified
Associated names	Hydroquinone, o-toluidine, xylidine, aniline condensate
Molecular weight (g/mol)	-
SMILES (canonical)	-

Additional chemical identity information

UVCB - this chemical is expected to contain phenyl and phenyl, phenyl and tolyl, tolyl and tolyl, tolyl and xylyl, and xylyl and xylyl substituted constituents.

CAS number	68953-84-4
CAS name	1,4-Benzenediamine, <i>N,N'</i> -mixed phenyl and tolyl derivatives
Molecular formula	Unspecified
Associated names	Hydroquinone, o-toluidine, aniline condensate
Molecular weight (g/mol)	-
SMILES (canonical)	-

Additional chemical identity information

UVCB - this chemical is expected to contain phenyl and phenyl, phenyl and tolyl, and tolyl and tolyl substituted constituents.

Relevant physical and chemical properties

Measured physical and chemical property data for seven chemicals (44PD, DPPD, IPPD, 7PPD, 77PD, PaTPD and 6PPD) were obtained from registration dossiers under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation in the European Union (EU), supplemented by two SIDS reports and the EPI Suite experimental database (ECHA CHEM n.d.-a to n.d.-g; OECD 2000; OECD 2004; US EPA 2017b). Data for two additional compounds (PaTaXPD and 8PPD) were obtained from previous NICNAS assessments (NICNAS 2001; NICNAS 2009).

Calculations for boiling point, vapour pressure, Henry's Law constants and soil adsorption coefficients (K_{oc}) were performed using EPI Suite (US EPA 2017a). The Henry's Law constants were calculated from the experimental water solubility and vapour pressure where both were available, otherwise the value from the bond method was used. K_{oc} values were estimated using the molecular connectivity index method. Calculated dissociation constant values (pKa) were estimated using the Chemaxon method available in QSAR Toolbox (LMC 2020).

Information for representative members of this evaluation are shown below. 44PD is a representative di-alkyl substituted *para*-phenylenediamine, 6PPD is a representative alkyl aryl substituted *para*-phenylenediamine and DPPD is a representative di-aryl substituted *para*-phenylenediamine:

	44PD	6PPD	DPPD
Physical form	Liquid	Solid	Solid
Melting point	17°C (exp.)	49.2°C (exp.)	143°C (exp.)
Boiling point	310–312°C (exp.)	370°C (calc.)	398°C (calc.)
Vapour pressure	0.026 Pa at 20°C (exp.)	3.6×10^{-3} Pa (calc.)	8.47×10^{-7} Pa (exp.)
Water solubility	32–62 mg/L (calc.)	1.1 mg/L (exp.)	0.15 mg/L (exp.)
Henry's law constant	1.8×10^{-3} Pa·m ³ /mol (calc.)	< 0.001 Pa·m ³ /mol (calc.)	1.47×10^{-3} Pa·m ³ /mol (calc.)
Ionisable in the environment?	Yes	Yes	Yes
pKa*	7.5 (exp.)	6.5 (calc.)	2.4 (calc.)
log K_{ow}	3.7 (exp.)	4.08 (exp.)	3.4 (exp.)
K_{oc}	1,312 L/kg (calc.)	23,000 L/kg (calc.)	52,000 L/kg (calc.)

*Basic pKa indicating deprotonation of the positively charged species to form a neutral species, not deprotonation of the neutral species to form a negatively charged species.

The physicochemical properties of chemicals in this evaluation are generally related to the substituent groups on the chemical. For example, log K_{ow} generally increases as the constituents increase in size. However, the aryl substituents have a reduced contribution to overall log K_{ow} value compared to alkyl substituents with similar numbers of carbon. DNPD, CPPD, 7PPD, 77PD, CCPD have log K_{ow} > 4.2, with the highest log K_{ow} of 6.4 estimated for DNPD. The constituents of PaTPD have measured log K_{ow} values in the range 3.3–4.6, while the constituents of PaTaXPD have measured log K_{ow} values in the range 3.5–4.6.

Introduction and use

Australia

Information reported to the former National Industrial Chemicals Notification and Assessment Scheme (NICNAS) under previous mandatory and/or voluntary calls for information indicates that the annual introduction volume of 6PPD was in the range of 100–1,000 tonnes. This volume does not account for the volume of 6PPD brought into Australia within articles such as tyres.

Information for two related chemicals is available from previous assessments under the NICNAS:

- PaTaXPD (CAS RN 68953-83-3) was assessed for use as an antioxidant in styrene-butadiene rubber, up to 0.75% by weight, for introduction volumes up to 10 tonnes/year (NICNAS 2001).
- 8PPD (CAS RN 15233-47-3) was assessed for use as a fuel antioxidant, added at 0.3 mg/L fuel, for introduction volumes up to 1 tonne/year (NICNAS 2009).

No further introductions of these two chemicals have been reported to the NICNAS or AICIS.

No specific information on industrial uses of the other chemicals in Australia has been identified. The uses of products or articles containing the other chemicals in this group are assumed to not significantly differ from uses reported internationally.

The chemical, DTPD (CAS RN 27417-40-9), is not likely to be commercially active in Australia under this chemical identity (AICIS 2022a). However, di-tolyl substituted *para*-phenylenediamines may be present as constituents in PaTPD or PaTaXPD (see **Chemical identity**).

International

Chemicals in this evaluation are antioxidants or antiozonants used in rubbers, plastics, oils and lubricants. Some of these chemicals are added to fuels.

These chemicals are added to natural and synthetic rubber during the manufacturing process to prevent cracking and improve their stability (OECD 2000; OECD 2004). These chemicals may be present within any rubber article, predominantly in tyres, but also in products such as transmission belts, hoses, cables and bushings (ECHA CHEM n.d.-c; ECHA CHEM n.d.-d; ECHA CHEM n.d.-e; ECHA CHEM n.d.-f).

Some of these chemicals are additives for acrylate polymers, and others are antioxidants added to petrol fuels and lubricants (ECHA CHEM n.d.-c; ECHA CHEM n.d.-d; ECHA CHEM n.d.-f; NCBI 2025; NICNAS 2009).

Data on manufacture, import and use volumes in other jurisdictions are available for many of chemicals in this evaluation. 6PPD has the highest reported volume in use globally, with PaTPD also having the next highest volumes reported.

Registration volumes under REACH (ECHA CHEM n.d.-a to n.d.-g) and aggregated volumes reported under the 2024 version of the US EPA CDR (US EPA 2024a) are presented below:

Chemical	REACH registration volume (tonnes)	2024 US EPA CDR Volume (tonnes)
6PPD	10,000–100,000	25,000–31,800
PaTPD	1,000–10,000	4,540–22,700
IPPD	1,000–10,000	113–181
77PD	1,000–10,000	249–454
44PD	100–1,000	454–1,130
7PPD	10–100	454–3,860
DPPD	1–10	< 34 (2023) 227–454 (pre-2023)

In the year 2006, 1,000–10,000 tonnes of PaTPD were imported into Canada (Government of Canada 2011).

Introduction volumes reported in Japan include 1–1,000 tonnes for each of 7PPD (MITI number 3-368), 44PD (MITI number 3-247) and DPPD (MITI number 3-145) (NITE n.d.).

Existing Australian regulatory controls

AICIS

1,4-benzenediamine, N,N'-mixed phenyl and tolyl and xylyl derivatives (PaTaXPD; CAS RN 68953-83-3) is listed on the Australian Inventory of Industrial Chemicals (the Inventory) with the following specific requirement to provide information as a term of the Inventory listing:

Obligations to provide information apply. You must tell us within 28 days if the circumstances of your importation or manufacture (introduction) are different to those in our assessment.

No specific controls are currently available for the other chemicals in this evaluation.

International regulatory status

United Nations

The chemicals in this group are not currently identified as Persistent Organic Pollutants (POP) (UNEP 2001), ozone depleting substances (UNEP 1987), or hazardous substances for the purpose of international trade (UNEP & FAO 1998).

OECD

The chemical 6PPD was sponsored by Japan under the Cooperative Chemicals Assessment Programme (CoCAP). The 18th Screening Information Data Set (SIDS) Initial Meeting Assessment (SIAM 18) in 2004 agreed that the chemical was a candidate for further work.

The report concluded that 6PPD possessed properties indicating a hazard for the environment, that further investigation on the identity and properties of the degradation products should be conducted and that an environmental risk assessment was recommended (OECD 2004).

The chemical IPPD was sponsored by the United Kingdom under CoCAP. The SIAM 10 in 2000 agreed that the chemical was a candidate for further work. The report noted the hazards of the chemical to the aquatic environment, and that the mechanism of toxicity remained unknown (OECD 2000).

United States of America

In 2024, the United States Environmental Protection Agency (US EPA) issued an advanced notice of proposed rulemaking in response to a petition to establish regulations to prohibit the manufacture, processing, use and distribution of 6PPD in tires under the Toxic Substances Control Act (TSCA) (US EPA n.d.-a). The public comment period on the notice closed in the first half of 2025.

In December 2024, the US EPA also finalised a rule under TSCA requiring manufacturers and importers to provide unpublished health and safety studies on 6PPD and 6PPD-q to the US EPA.

Canada

In 2011, Environment Canada and Health Canada completed a screening risk assessment of PaTPD and a related di-aryl substituted *para*-phenylenediamine (CAS RN 68478-45-5) under the Challenge initiative of the Chemicals Management Plan (Government of Canada 2011).

The risk assessment considered estimates of environmental releases to wastewater from industrial processes and estimates releases from consumer uses of tyres, based on total volumes of chemical for particular uses. Environment Canada and Health Canada concluded that some predicted environmental concentrations (PECs) of PaTPD in Canada were above the predicted no effect concentration (PNEC), indicating that PaTPD had the potential to cause ecological harm in Canada.

In June 2019, PaTPD was added to Schedule 1 of the Canadian Environmental Protection Act, 1999 (Government of Canada n.d.-a; Government of Canada n.d.-b).

Japan

None of the chemicals are classified as Priority Assessment Chemical Substances (PACS) under Japan's Chemical Substances Control Law. However, PaTPD is a Class I specified chemical substance and 6PPD a Type III Monitoring Chemical Substance (NITE n.d.).

Environmental exposure

The chemicals in this evaluation will be released to the soil, water and partition to sediment compartments through their industrial uses.

The main environmental release pathway for the chemicals is through rubber particles released during tyre wear. Tyre particles are continuously shed from tyres during use, and the particles initially fall on the road or onto soils next to roads (Mayer et al. 2024). Tyre

particles can be airborne and transported away from the sources (Johannessen et al. 2025; Wu et al. 2020), but they are not expected to be mobilised into water surfaces until rainfall events create water flows that can move a fraction of tyre particles into waterways (Müller et al. 2022).

The chemicals are not bound within the rubber and migrate to the surface of rubber products and rubber particles (Zoroufchi Benis et al. 2023). Some fraction of the chemicals may then degrade through oxidation or ozonation (see **Degradation**). Once on the surface, the chemicals or their degradants are available to leach either directly into stormwaters, or into waterways once the rubber particle containing them has been carried to a river or other waters. While only a small fraction of chemicals in the rubber may leach into water (Müller et al. 2022), the release from tyre wear particles is considered a significant source of the chemicals and their degradants in the environment due to constant releases from large volumes of tyres.

Simulation studies on recycled tyre products, such as rubber crumb or rubber mulch, have demonstrated that 6PPD degradants and other rubber related substances will leach from rubber particles into water and rainwater (Bryshun et al. 2026; Srivastava et al. 2026). This indicates that releases of these chemicals and their degradants may also occur from the use of recycled tyre products. Depending on the location of use, these chemicals and degradants will drain to nearby soils and be immobile or to stormwater.

Road runoff and stormwater are not treated in sewage systems in Australia. During significant rainfall events, rubber particles and any leached chemicals will be carried into the stormwater systems or released directly to nearby waterways (Rauert et al. 2022b). Environmental monitoring information from Canada indicates that the highest concentrations of 6PPD degradants in urban waters may occur during or after rainfall events (Black et al. 2025; Johannessen et al. 2022), indicating increased environmental exposure during these events.

Manufacturing of rubber products may result in minor emissions that are expected to go to sewage and be treated in sewage treatment plants (STPs) (NICNAS 2001). Similarly, uses in lubricants and oils are only expected to result in minor releases to STPs or disposal to landfill. No release of chemicals to the environment from the use in fuel is likely as these chemicals are expected to be consumed during combustion.

Environmental fate

Chemicals in this evaluation are expected to be released into the soil and water and partition to sediment compartments. In these compartments they will be transformed by abiotic processes, mainly hydrolysis and oxidation or ozonation, to form several degradation products.

Dissolution, speciation and partitioning

The chemicals have measured or estimated basic pKa values that range from 2.2 for DNPD to 7.5 for 44PD. Di-aryl substituted *para*-phenylenediamines are predicted to have basic pKa values below 4, indicating that they will predominately exist in the neutral form under environmental conditions. Di-alkyl and alkyl aryl substituted *para*-phenylenediamines generally have predicted or measured basic pKa values closer to 7, indicating that these chemicals will exist in both neutral and protonated forms under environmental conditions.

These chemicals have solubilities ranging from very slightly to moderately soluble and volatility ranging from very slight to moderately volatile. Calculated Henry's law constants for

chemicals in this group range from negligible to 0.875 Pa.m³/mol, indicating very slight to moderate potential to volatilise from surface waters and moist soil, in their neutral form. These chemicals are not expected to be volatile from water when protonated.

Based on their calculated Koc values, four substances (33PD, 44PD, IPPD, CCPD) have medium to slight mobility in soil (Koc values 360–4,300 L/kg), while others are immobile in soil (Koc > 5,000 L/kg).

The Level III Fugacity model with equal emissions into water and soil, estimates partitioning to the soil (51–81%), water (3–20%) and sediment (1–40%), with negligible proportions to air (< 0.01%) for all chemicals in this group, except for the more hydrophobic DNPD. The latter chemical will partition mainly between soil (30%) and sediment (69%) (US EPA 2017a).

In road runoff, the majority (> 90%) of 6PPD and the degradant 6PPD-q are present in the particulate phase rather than in solution (Seiwert et al. 2022), suggesting that other chemicals in this evaluation may also strongly associate with particulate in environmental waters.

Degradation

Available evidence indicates that the chemicals will transform within threshold timeframes (DCCEEW 2022) and are not persistent.

The degradation of the chemicals is dominated by abiotic pathways. Rapid transformation due to hydrolysis and photolysis is observed for most of the chemicals across a variety of degradation tests. However, mineralisation is typically limited. Di-aryl substituted *para*-phenylenediamines, such as DPPD, DNPD, or the constituents of PaTPD and PaTaXPD, are more resistant to hydrolysis, but still decompose with half-lives shorter than 60 days.

Available information suggests that quinone degradants of all the chemicals only form under ozonation or oxidation conditions.

Hydrolysis

Hydrolysis targets the secondary amine functionality in the chemicals resulting in decomposition (Di et al. 2022; Xu Y et al. 2025).

Hydrolysis is rapid for the chemicals with either one or two alkyl substituents. The typical half-lives for these *para*-phenylenediamines are shorter than 1 day. Di-aryl substituted *para*-phenylenediamines are more resistant to hydrolysis.

Measured hydrolysis half-lives at pH 7 include (Di et al. 2022; ECHA CHEM n.d.-b; ECHA CHEM n.d.-e; ECHA CHEM n.d.-g; OECD 2000; OECD 2004; Platt et al. 2025; Xu S et al. 2024; Xu Y et al. 2025):

- 3.9–11 hours for IPPD
- 5.3 hours for 44PD
- 4.3–14 hours for 6PPD
- 29.5 hours (1.2 days) for DNPD
- 46.5–970 hours (1.9–40.4 days) for DTPD
- 1,087 hours (43 days) for DPPD.

Other than DPPD, the estimated hydrolysis half-life for all substituted *para*-phenylene diamines is below 10 days (Xu Y et al. 2025), including for various tolyl or xylyl substituted constituents of PaTPD and PaTaXPD.

Hydrolysis forms amines and alcohol derivatives of the substituents, along with amine or hydroxyl *para*-substituted phenols.

Phenyl substituted *para*-phenylenediamines, such as 6PPD or IPPD, form 4-hydroxydiphenylamine (4-HDPA; CAS RN 122-37-2) and an alkyl amine under the dominant hydrolysis pathway (Di et al. 2022; Xu Y et al. 2025), plus phenol (CAS RN 108-95-2) and 4-aminophenol (CAS RN 123-30-8) from hydrolysis of the phenyl bond. 4-HDPA then undergoes further hydrolysis (half-life 3.33–9.11 hours) to form a mixture of p-hydroquinone (CAS RN 123-31-9), and aniline (CAS RN 62-53-3).

DNPD hydrolysis forms a mixture of 2-naphthol and 2-naphthaleneamine along with 4-aminophenol (Xu Y et al. 2025).

No information on the hydrolysis products of non-aryl substituted *para*-phenylenediamines, such as 44PD, is available. Considering the known mechanism for other *para*-phenylenediamines (Xu Y et al. 2025), it is likely that a mixture of amines and alcohol derivatives of the alkyl substituents will be formed, along with a mixture of p-hydroquinone and 4-aminophenol.

The formation of quinone degradants, such as 6PPD-q, is only observed under acidic conditions (pH 4) and is not expected to occur by hydrolysis under typical environmental conditions (Di et al. 2022).

Oxidation / Ozonation

Oxidation and ozonation are the key transformation pathways that can result in the formation of highly toxic quinone degradants, such as 6PPD-q.

Mechanistic studies on oxidation and ozonation are only available for 6PPD and indicate two main transformation pathways for phenyl substituted *para*-phenylenediamines (Seiwert et al. 2022; Zhao et al. 2023):

- Decomposition resulting in the formation of an alkylamine and a mixture of amine, nitroso, and nitro 4-substituted diphenylamines.
- Rearrangement to accommodate oxygen atoms resulting in the formation of substituted *para*-phenylenediamine -quinones or amine-oxide *para*-phenylenediamine derivatives.

Transformation of 6PPD to 6PPD-q has been observed both through oxidation of 6PPD in water and ozonation of 6PPD bound to particles, including on the surface of rubber (Zhao et al. 2023).

Average molar yields of 6PPD-q have been estimated between ≤1% and 9.7% for direct exposure of 6PPD to ozone (Hu et al. 2022; Zhao et al. 2023), and up to 8% for 6PPD in snow melt (Seiwert et al. 2022).

While mechanistic studies are not available for the chemicals other than 6PPD, the formation of quinone degradants of the other chemicals, including various di-alkyl and di-aryl

substituted *para*-phenylenediamines, has been confirmed through detections in the environment (Zeng L et al. 2023; Zhou L-J et al. 2024).

Photolysis

The chemicals react photolytically in both the atmosphere and surface waters to form various degradants.

The photolytic half-life for 6PPD in air is estimated at 1 h (OECD 2004) and half-lives between 0.4 h and 3.1 h are estimated for others (ECHA CHEM n.d.-b; ECHA CHEM n.d.-c; ECHA CHEM n.d.-d; ECHA CHEM n.d.-e; OECD 2000).

Measured photolytic half-lives in pure water under simulated sunlight irradiation and UV filters range from 3.6 min to 19.3 h for IPPD (Wang C et al. 2024) and between 2.4–17.5 hours for 6PPD (Kuntz et al. 2026; Platt et al. 2025). DPPD, which is stable in aqueous solutions under dark conditions, is photolytically degraded with a half-life of 14.4 minutes in pure water (Wang C et al. 2024). Aqueous photolysis is enhanced by the presence of dissolved organic matter in environmental waters (Platt et al. 2025; Redman et al. 2023), whereas photolysis is reduced with increasing pH (Li C et al. 2023).

Major photolytic products of 6PPD are aniline, 4-HDPA and 4-aminodiphenylamine (CAS RN 101-54-2) (Li C et al. 2023). Photolytic degradation of 6PPD to form 6PPD-q has also been observed at molar yields of 1 to 3% (Li C et al. 2023; Zhou Y et al. 2023).

Simulation studies in river water

Studies on the degradation of the chemicals in natural waters indicate rapid transformation of *para*-phenylenediamines with one phenyl substituent and slower transformation for di-aryl and di-alkyl substituted *para*-phenylenediamines. However, overall mineralisation is limited for all substituted *para*-phenylenediamines under study conditions.

An OECD TG 309 study on IPPD using German river water indicated that the transformation of IPPD is rapid, but mineralisation is limited (ECHA CHEM n.d.-g). IPPD was transformed into other products with a half-life of 16.7–23.3 hours at 12°C, with 90% transformation observed under 78 hours (3.3 days). Initial degradants observed in the first two days of the study included N-Phenyl-p-benzoquinone imine (NPQI; CAS RN 2406-04-4) and 4-HDPA. These degradants further degraded into more polar metabolites, including 1,4-cyclohexanedione (CAS RN 637-88-7), and were not present at the end of the 12-day study. Despite the rapid transformation, only 10.9% of the initial IPPD was mineralised into CO₂.

Slower transformation was observed in an OECD TG 309 study on PaTPD using German lake water (ECHA CHEM n.d.-e). Transformation half-lives of 11.1–29.6 days were calculated. Mineralisation of PaTPD was below 5% in all replicates. Transformation of PaTPD into a diimine species was observed to be immediate on day 0 and was not considered in half-life determination.

Studies on IPPD and 6PPD in Mississippi River water observed rapid transformation regardless of the biological activity of the water. The transformation half-life of 6PPD at 24°C was 2.9 hours in active river water, 3.9 hours in sterile river water and 6.8 hours in sterile deionised water. No formation of 6PPD-q was observed in this study (ECHA CHEM n.d.-f). The transformation half-life of IPPD at 24°C was 2.5 hours in active river water, 5.4 hours in sterile river water and 11.3 hours in sterile deionised water (ECHA CHEM n.d.-g). No

analysis of transformation products or mineralisation was reported alongside either of these results.

Another study dosed samples of river water from Hong Kong with used tyre wear rubber particles and measured the degradation kinetics of several of the chemicals (Xu S et al. 2024). Estimated half-lives for IPPD, CPPD and 6PPD were less than 1 day, whereas those of 77PD, DPPD, DNPD and DTPD were 8, 12.9, 16.4 and 40.4 days, respectively. A variety of hydrolysis and biotic transformation products were reported. The presence of quinone degradants including 6PPD-q, 77PD-q and DPPD-q were also reported by the authors. However, it is unclear what contribution continual leaching from the used tyre wear particles had on the observed concentrations.

Ready biodegradation

Results of ready biodegradation studies on the chemicals indicate that overall mineralisation is limited, despite transformation occurring.

Results for ready biodegradation studies are available for a wide range of substituted *para*-phenylenediamines (ECHA CHEM n.d.-c; ECHA CHEM n.d.-d; ECHA CHEM n.d.-e; ECHA CHEM n.d.-f; NICNAS 2001; OECD 2000; OECD 2004), and include:

- 2% mineralisation of 6PPD in 28 days in an OECD TG 301C study
- 7.2% mineralisation of 6PPD in 32 days in a study similar to OECD TG 301B
- 18.9% mineralisation of IPPD in 32 days in a study similar to OECD TG 301B
- 12% mineralisation of 77PD in 28 days in an OECD TG 301C study
- 0% CO₂ evolution for 7PPD in 35 days under an ASTM ultimate biodegradability test
- <1 % mineralisation of PaTPD in 28 days in an OECD TG 301F study
- 1.72% mineralisation of PaTaXPD in an OECD TG 301B study.

While limited mineralisation was observed in the OECD TG 301C study on 6PPD (OECD 2004), analysis of the test material concentrations indicated that 92% of the parent substance had decomposed into smaller degradants. Identified degradants included:

- NPQI (CAS RN 2406-04-4)
- 1,3-Dimethylbutylamine (CAS RN 108-09-8)
- 4-HPDA (CAS RN 122-37-2)
- p-benzoquinone (CAS RN 106-51-4)
- Aniline (CAS RN 63-53-3).

Two of these degradants (p-benzoquinone and aniline) are readily biodegradable (AICIS 2022b; NICNAS 2013). 4-HPDA undergoes hydrolysis to biodegradable compounds (see **Hydrolysis**), and the others are vulnerable to biodegradation. However, this complete degradation has not been observed under the test conditions of the parent chemicals.

A non-guideline degradation study investigated the degradation of three of the chemicals in the presence of activated sludge (Han et al. 2025). The study also investigated the degradation of four common transformation products. All tested chemicals underwent complete transformation within 14 days, with estimated half-lives of 0.2 days for 6PPD, 0.6 days for IPPD and 1 day for DPPD.

Simulation studies in soils and sediments

Available information indicates that the chemicals are expected to rapidly transform in soils under aerobic conditions but are slower to degrade under anaerobic conditions.

The degradation of 6PPD was rapid in aerobic soils but slower in anaerobic soils and sediments in a study analogous to OECD TG 307 and 308 (Shen et al. 2025). The half-life of 6PPD was shorter than 2 days in both tested soils. While degradation was faster in the non-sterilised soil, the results strongly indicate that aerobic degradation in soil is mostly abiotic. In contrast, no degradation of 6PPD was observed in soils altered to anaerobic conditions after 60 days. In sediment tests, 6PPD was transformed with a half-life of 51.4 days. Since no degradation was observed in the test with sterilised sediment, this result indicates the degradation in sediment was driven by biotic degradation. A variety of metabolites were identified, including 4-HDPA and NPQI. No formation of 6PPD-q was identified.

Similarly, in an experiment with paddy soils dosed with tyre particles, concentrations of 6PPD reduced in non-sterilised soils under aerobic and anaerobic (flooded) conditions (approximate half-lives below 22 days). 6PPD concentrations either did not significantly reduce or reduced more slowly (half-life approximately 45 days), in sterilised soils under both aerobic and anaerobic conditions (Xu Q et al. 2023).

Aerobic degradation of 7PPD is also rapid, with half-lives shorter than 2 days in various soils under a study that followed OECD TG 307 (ECHA CHEM n.d.-c). However, mineralisation was limited with only 4.1–8.9% of applied radioactivity converted into CO₂ after 56 days. A dominant proportion of applied radioactivity, 76.4–84.8%, was bound to soil and considered to be non-extractable and not bioavailable. 7PPD was resistant to degradation under anaerobic conditions, with an estimated half-life of 90 days in the anaerobic test (ECHA CHEM n.d.-c). The only metabolite identified across the aerobic and anaerobic tests was 1-N-(5-methyl-hexan-2-yl)-4-N-phenylcyclohexa-2,5-dione-4,4-diimine (7QDI).

Degradation of quinone degradants

Limited information is available regarding degradation of the quinone degradants.

The degradant 6PPD-q is stable to hydrolysis in the pH range 5 to 9 under dark conditions, with only 26% degradation after 47 days (Hu et al. 2023). Degradation of 6PPD-q is increased when exposed to sunlight, with observed half-lives of 3.9 hours and >9.2 hours (Kuntz et al. 2026; Platt et al. 2025). In natural waters, reported half-lives of 6PPD-q are:

- 12.8 days in river water under dark conditions (Di et al. 2022)
- 17 to 22 hours in lake waters at ambient temperature (20 °C) under direct exposure to sunlight (Redman et al. 2023).

In an experiment with paddy soils dosed with tyre particles, concentrations of 6PPD-q reduced in non-sterilised soils under aerobic and anaerobic (flooded) conditions (approximate half-lives 15–31 days). No significant removal of 6PPD-q was observed in the sterilised soil replicates, indicating that the degradation was driven by soil microorganisms (Xu Q et al. 2023).

In a test with tyre wear rubber particles, removal of 6PPD-q and IPPD-q in wastewater under activated sludge conditions were 99% and 100%, respectively after 28 days. Calculated half-lives were 3 days for 6PPD-q and 1.9 days for IPPD-q (Han et al. 2025).

Bioaccumulation

Available information indicates that DNPd, DTPD, and some constituents of PaTPD and PaTaXPD meet the thresholds for bioaccumulation. These chemicals or constituents have experimental bioconcentration factors (BCFs) and log K_{OW} values that exceed thresholds for bioaccumulation (DCCEEW 2022).

Estimated bioaccumulation information for 77PD and CCPD is mixed, with some predicted BCF or bioaccumulation factor (BAF) values exceeding thresholds and some predicted BCF values below thresholds. The currently available information is insufficient to categorise these chemicals as meeting the threshold for bioaccumulation (DCCEEW 2022).

The remaining chemicals do not meet thresholds for bioaccumulation due to experimental BCFs, estimated BCFs and BAFs, or log K_{OW} values below the thresholds for categorisation (DCCEEW 2022).

Fields studies indicating elevated BAFs or trophic magnification for some chemicals have been identified. However, sample handling practices raise uncertainties in the BAF values, while the impact of high industrial activity raises uncertainties in the trophic magnification measurements. As a result, the highest weight of evidence has been placed on the experimental BCF values that are available, along with considerations of estimated BCF and BAF and measured or estimated log K_{OW} values.

Bioconcentration and bioaccumulation factors

Experimental information indicates that DNPd and DTPD have BCF values above 2,000 L/kg, exceeding bioaccumulation thresholds. Some constituents of PaTPD and PaTaXPD have experimental BCF values above 2,000 L/kg, exceeding bioaccumulation thresholds. All other chemicals are not considered to meet bioaccumulation thresholds or have insufficient information to categorise the chemicals as meeting bioaccumulation thresholds. These chemicals have experimental or estimated BCF and BAF values below 2,000 L/kg, or log K_{OW} values below 4.2. Some field studies report BAF values above thresholds for some chemicals. However, the methodology of these studies may result in the reported values being overestimated.

Based on measured or experimental log K_{OW} values above 4.2, DNPd, DTPD, CPPD, 7PPD, 77PD, CCPD, some constituents of PaTPD and PaTaXPD have increased potential for bioaccumulation.

Measured BCFs in aquatic organisms for several substituted *para*-phenylenediamines are above 2,000 L/kg for DNPd, DTPD, and constituents of PaTPD and PaTaXPD, and below 2,000 L/kg for 8PPD and DPPD.

Reported BCF results from OECD TG 305 studies performed by MITI/Japan on common carp (*Cyprinus carpio*) include (NITE n.d.):

- 1,500–1,700 L/kg for 8PPD
- 260–1,400 L/kg for DPPD
- 1,000–1,400 L/kg in the high concentration test for DNPd
- 1,700–2,600 L/kg in the low concentration test for DNPd
- 3,760–14,600 L/kg for DTPD
- 4,210–15,200 L/kg for tolyl and xylyl substituted *para*-phenylenediamines
- 3,340–14,600 L/kg for xylyl and xylyl substituted *para*-phenylenediamines

An experimental BCF value of 1,320 L/kg for DPPD is also reported in the training data set for the BCFBAF program in EPI Suite (US EPA 2017a).

No experimental BCF data is available for all other chemicals in this evaluation, including CPPD, 7PPD, 77PD and CCPD.

Bioaccumulation estimates using the Arnot-Gobas method predict BCFs and BAFs below 2,000 L/kg for CPPD and 7PPD (US EPA 2017), indicating that these chemicals are unlikely to meet bioaccumulation thresholds. Arnot-Gobas estimates for 77PD and CCPD result in BCFs below 2,000 L/kg, with some BAFs above 2,000 L/kg (US EPA 2017). Catalogic BCF base line predictions for 77PD and CCPD also suggest that the BCF for these chemicals will be below 2,000 L/kg, with metabolism and chemical size predicted to be key factors in mitigating bioaccumulation (LMC 2015). As such, 77PD and CCPD are not expected to meet thresholds for bioaccumulation.

All other chemicals in the evaluation (IPPD, 44PD, 4PPD, 6PPD, 33PD) have measured or estimated log K_{OW} values below 4.2 and are unlikely to meet bioaccumulation thresholds for aquatic organisms.

Field studies have measured log BAF values above the bioaccumulation threshold (log BAF > 3.3) for IPPD (range 3.2 to 4.6), 6PPD (range 2.7 to 4.7), DPPD (range 3.4 to 5.2) and DTPD (4.4) in bivalves, sea cucumber, snails, crustaceans (Liu et al. 2025; Wei et al. 2024; Zeng J et al. 2025). None of the quinone degradants were observed to have log BAFs above the regulatory threshold in these studies. While these studies indicate BAFs above the threshold value, methodological limitations associated with water sample handling indicate that the results are not considered reliable.

Two of the studies (Liu et al. 2025; Wei et al. 2024) filtered the water samples before analysis. Considering the K_{OC} values of the targeted chemicals are above 4,000 L/kg, a considerable proportion of chemical will be adsorbed to particulate matter. Discarding the filtered fraction may have underestimated the bioavailable concentrations of the chemicals in water and overestimated the BAF values.

The other study (Zeng J et al. 2025) did not report acidifying samples upon collection to prevent degradation of the chemicals in the samples. Many of the chemicals, including 6PPD and IPPD, are readily hydrolysable (see **Degradation**) and so collection techniques that fail to account for abiotic degradation will underestimate the concentration of the chemicals in the environment and overestimate the BAF values.

Trophic magnification

Three studies measured the concentrations of some of the chemicals in biota to investigate trophic magnification of the chemicals. While trophic magnification factors (TMFs) above 1 were calculated for IPPD, DPPD, DTPD and DPPD-q in at least one study, a low weight of evidence has been placed on these studies.

All three studies were performed in areas heavily affected by industrial activity. The Pearl River Estuary receives waters from very highly industrialised and urbanised regions in the Guangdong-Hong Kong-Macau area (Wei et al. 2024). The Nandu River reportedly runs through China's largest base of rubber production (Liu et al. 2025). It is unclear how the observed trophic magnification values could be influenced by periodic high concentration flows, especially for short-lived chemicals such as IPPD.

One study measured IPPD, 6PPD, DPPD, DTPD and 6PPD-q in biota in the Pearl River Estuary (Wei et al. 2024). All chemicals were detected in at least one sample. No significant trophic magnification was reported for these chemicals.

Another study within a mangrove within the Pearl River Estuary measured concentrations of IPPD, 6PPD, CPPD, DPPD, DNPd, 77PD, DTPD and their respective quinones in biota (Zeng J et al. 2025). All chemicals were detected in at least one species, except for 77PD which was not detected despite 77PD-q being detected. Significant TMFs above 1 were reported for IPPD, DPPD, DTPD and DPPD-q.

One study on the Nandu River Estuary measured concentrations of IPPD, 6PPD, CPPD, DPPD, DTPD and their respective quinones in biota (Liu et al. 2025). Detections were reported for IPPD, 6PPD, DPPD, 6PPD-q and IPPD-q. A significant TMF above 1 was reported for IPPD. However, one of the key species (*Acanthopagrus latus*) in the TMF derivation for IPPD was a carnivorous fish species with measured trophic level below the reference trophic level of zooplankton. This trophic level measurement is unusual as it suggests that a predator species has lower trophic level than a primary consumer species. This key species has a large influence on the trophic magnification trend analysis, and the trend or its statistical significance is not expected to hold if this species were excluded from the analysis or adjusted to a trophic level reflective of other carnivorous fish.

Environmental transport

The chemicals are not expected to undergo long range transport based on their short half-lives in both the atmospheric and aquatic environments.

Predicted environmental concentration (PEC)

Various PECs have been considered for the chemicals and degradants in this evaluation. As the most serious adverse effects related to the chemicals or their degradants are expected to occur over short-time frames (see **Effects on Aquatic Life**), maximum values from monitoring studies have been conservatively considered in PEC derivation, rather than typical average or median values.

Based on international monitoring information the PECs for the chemicals in water are:

- 2.7 micrograms per litre (µg/L) for di-alkyl and alkyl aryl substituted *para*-phenylenediamines
- 0.16 µg/L for di-aryl substituted *para*-phenylenediamines.

The previous PEC for the use of PaTaXPD in rubber manufacturing (0.072 µg/L) (NICNAS 2001) is lower than the PEC derived for di-aryl substituted *para*-phenylenediamines for all uses of the chemicals. No further consideration of the previous PEC for rubber manufacturing is required.

The PEC in water for the degradant 6PPD-q is 0.088 µg/L based on Australian monitoring information. This is considered worst-case for all quinone degradants as 6PPD is likely introduced in the highest volumes.

The PECs for sediment were only derived for the chemicals with sufficient toxicity information for risk characterisation. The PEC for 6PPD in sediments is 468 micrograms per kilogram dry weight (µg/kg dw) based on international monitoring information. The PEC for 6PPD-q in sediment is 27 µg/kg dw based on international monitoring information.

Substituted *para*-phenylenediamines in surface waters and effluents

No Australian monitoring information on chemicals in environmental waters is available. Globally, concentrations of these chemicals vary widely in different environmental waters with concentrations peaking during rainfall events.

Maximum concentrations of 6PPD in runoff and surface waters are generally below 1 µg/L and average concentrations are generally below 0.1 µg/L across a variety of studies (Brown et al. 2026; Yang W et al. 2024; Zhang et al. 2024; Zhao et al. 2023; Zhu et al. 2024). The highest 6PPD concentrations are typically found in urban runoff, with measurements up to 2.7 µg/L reported in samples from Hong Kong and 12.2 µg/L reported in samples from New York State, USA (Cao et al. 2022; Li Z-M et al. 2025). 6PPD has been measured in surface waters at concentrations up to 1.35 µg/L in lake water in New York State (Li Z-M et al. 2025) and up to 0.38 µg/L in urban waterways during rainfall events in Canada and the USA (Brown et al. 2026; Soucek et al. 2025). Maximum 6PPD concentrations in sewage treatment plant (STP) effluents are generally below 0.02 µg/L (Cao et al. 2023; Li Z-M and Kannan 2024; Xu S et al. 2025) except in locations where STPs receive stormwater for treatment, such as Germany (Seiwert et al. 2022).

In comparison, maximum runoff concentrations are below 0.3 µg/L for the other chemicals in this evaluation, with concentrations up to 0.27 µg/L for IPPD, 0.16 µg/L for DTPD and 0.14 µg/L for DNPD (Cao et al. 2022; Liu Y-H et al. 2024; Xu S et al. 2024; Zhang H-Y et al. 2023). Similarly, maximum concentrations of the other chemicals in surface waters are typically below 0.2 µg/L (Brown et al. 2026; Geng et al. 2025; Liu Y-H et al. 2024; Zeng J et al. 2025), except for DNPD which has been measured at concentrations up to 0.34 µg/L in an urban lake in China under snow-affected conditions (Zhang et al. 2024).

The chemical with the highest measured environmental concentrations is 6PPD and so 6PPD is representative of the worst-case environmental concentrations for the di-alkyl or alkyl aryl substituted *para*-phenylenediamines in this evaluation. As such, the reasonable worst-case PEC for di-alkyl or alkyl aryl substituted *para*-phenylenediamines in water is 2.7 µg/L, based on maximum 6PPD concentrations measured in runoff in Hong Kong. This value is considered conservative, as it is greater than the average measured 6PPD concentrations in water monitoring studies across a variety of countries and location types, and greater than the maximum 6PPD concentrations in most monitoring studies. The maximum 6PPD value from New York State was not chosen as it greatly exceeded all other values and its relevance to Australian conditions was uncertain.

The PEC for the di-aryl substituted *para*-phenylenediamines in this evaluation is 0.16 µg/L, based on the highest value for DTPD in runoff. This value is the highest measured value for any of the di-aryl substituted *para*-phenylenediamines in this evaluation, other than the reported measurements for DNPD in an urban lake, and is conservative. The DNPD concentration was not considered to be relevant as snow conditions in urban locations are not typical Australian conditions.

Degradant quinones in surface waters and effluents

Concentrations of degradants have been measured in waters globally. Some quinone degradants, such as 6PPD-q, are regularly reported at concentrations that exceed parent concentrations in the same studies.

The PEC for 6PPD-q in water is 0.088 µg/L based on the maximum 6PPD-q concentration measured in Australia, as this value is the highest environmental concentration measured under Australian conditions. However, it is noted that higher maximum concentrations for

6PPD-q have been observed internationally. Refinement of the PEC for 6PPD-q may be required as further Australian monitoring information becomes available.

Australian data are available only for 6PPD-q in urban surface waters in Brisbane, where maximum concentrations up to 0.088 µg/L in both runoff and urban waterways have been reported across the two studies (Rauert et al. 2022a; Rauert et al. 2022b). This maximum value was observed in an urban creek during a storm event, in a location 160 metres downstream of a major Brisbane highway.

Higher concentrations of 6PPD-q have been observed in runoff internationally. Maximum 6PPD-q concentrations from the Greater Bay Area, China, include:

- 2.43 µg/L in Hong Kong (Cao et al. 2022),
- 1.56 µg/L across Huizhou and Dongguan (Zhang H-Y et al. 2023)
- 0.94 µg/L in 43 samples across the various Greater Bay Area cities (Liu Y-H et al. 2024).

In the USA, analysis of runoff waters from Seattle, San Francisco and Los Angeles indicated 6PPD-q concentrations up to 2.3 µg/L (corrected value) (Tian et al. 2021), while concentrations up to 1.74 µg/L were measured in runoff in New York State (Li Z-M et al. 2025).

Elevated maximum concentrations of 6PPD-q in surface waters have also been reported globally. In North American waters, maximum 6PPD-q concentrations of 2.85 µg/L were measured in a Toronto river during a storm event (Johannessen et al. 2022) and concentrations up to 0.54 µg/L in lake water in New York State (Li Z-M et al. 2025).

In China, a maximum 6PPD-q concentration of 0.99 µg/L was detected in the Guangdong River after a stormwater discharge event (Ren et al. 2024), while maximum concentrations up to 0.20 µg/L were measured in urban rivers across 45 major Chinese cities (Geng et al. 2025).

The maximum concentrations of the quinone degradants for chemicals other than 6PPD-q in runoff or surface water include 0.95 µg/L for IPPD-q, 0.82 µg/L for DTPD-q, and 0.35 µg/L for DPPD-q (Cao et al. 2022; Geng et al. 2025; Liu Y-H et al. 2024).

Substituted *para*-phenylenediamines and quinone degradants in sediment

No Australian sediment monitoring information is available. Internationally, sediment surveys indicate that concentrations vary depending on location and the specific chemical.

Two extensive sediment studies from China are available. These two studies cover a broad range of locations across China, covering locations with differing proximity to urban and industrial centres. These studies have been chosen to inform worst-case concentrations for sediment in Australia, as the level of industrialisation and urbanisation in some sampled areas of China exceed Australian conditions. The PEC for 6PPD in sediments is 468 µg/kg dw based on the highest concentration of 6PPD in sediments across these two studies. The PEC for 6PPD-q in sediments is 27 µg/kg dw based on the maximum concentration of 6PPD-q across these two studies.

One study measured sediment concentrations of substituted *para*-phenylenediamines and their quinone degradants at 85 locations from the Pearl River Delta, the Pearl River Estuary and the South China Sea (Zeng L et al. 2023). The highest sediment concentrations were

found in the sediments of urban rivers, with maximum 6PPD concentrations up to 468 µg/kg dw and median 6PPD concentrations of 14.4 µg/kg dw. 6PPD sediment concentrations in areas other than urban rivers were all below 12 µg/kg dw. Maximum sediment concentrations of other chemicals, including IPPD, DPPD and DNPd, were all below 70 µg/kg dw in urban rivers and below 10 µg/kg dw elsewhere.

Another study measured sediment concentrations of substituted *para*-phenylenediamines and their quinone degradants in 118 Chinese lakes (Zhou L-J et al. 2024). The highest maximum concentrations in sediment were found for CPPD at 741 µg/kg dw and DTPD at 539 µg/kg dw. In comparison, the maximum 6PPD sediment concentration was 27 µg/kg dw. Mean concentrations for 6PPD, CPPD, DNPd, DPPD, DTPD and IPPD were all below 10 µg/kg dw.

The concentrations of quinone degradants were below 25 µg/kg dw in both studies, with maximum values of 18.2–23 µg/kg dw for 6PPD-q, 17.8 µg/kg dw for 77PD-q and 11 µg/kg dw for CPPD-q (Zeng L et al. 2023; Zhou L-J et al. 2024). The highest median concentration of a quinone degradant was reported for 6PPD-q at 9.0 µg/kg dw (Zeng L et al. 2023).

Environmental effects

Effects on the atmosphere

The chemicals in this group are not expected to contribute to global warming.

Although the chemicals can react with ozone in the lower atmosphere to form quinone degradants, their low volatility and rapid transformation half-lives limit atmospheric exposure and transport. As a result, they are not expected to reach the stratosphere in significant quantities (Kuntz et al. 2026) and are; therefore, not expected to affect the stratospheric ozone layer.

Effects on aquatic Life

All chemicals in this evaluation are either toxic to aquatic organisms or degrade into products that are toxic to aquatic organisms.

Ecotoxicity information is available for many of the chemicals in this evaluation, as well as for key degradants including:

- 6PPD-q
- 4-aminophenol (OECD 2010)
- p-hydroquinone (AICIS 2022b)
- aniline (NICNAS 2013).

Alkyl aryl and di-alkyl substituted *para*-phenylenediamines readily undergo abiotic degradation under typical pH conditions (see **Degradation** section) and this makes toxicity testing of these substances difficult to assess. The ecotoxicity for these chemicals is due to a combined effect of the parent chemical and the degradation products formed. As di-aryl substituted *para*-phenylenediamines degrade more slowly, the parent chemicals are expected to have a greater influence on their overall toxicity. The collated information indicates that alkyl aryl substituted *para*-phenylenediamines have the highest toxicity to fish, while di-aryl substituted *para*-phenylenediamines may have the highest toxicity to algae in

comparison. As acute endpoint values below 1 mg/L are observed for at least one trophic level for a wide range of chemicals in this evaluation, read-across indicates that all chemicals in this evaluation will have acute toxicity endpoints below 1 mg/L.

The highly toxic degradation product 6PPD-q is not observed to form during hydrolysis at environmentally relevant pH values (Di et al. 2022) and is therefore not expected to form during standard ecotoxicity tests on 6PPD. The difference in fish toxicity endpoints between 6PPD and 6PPD-q highlight this phenomenon.

A large body of recent literature has investigated the significant toxicity of 6PPD-q, particularly species-specific sensitivity in fish and its potential mode of action. Salmonid species, including salmon and trout, have been found to be the most sensitive to the effects of 6PPD-q (Brinkmann et al. 2022; González-Vázquez et al. 2025).

Toxic effects occur rapidly with most mortality occurring within 24 hours of exposure (Lo et al. 2023; Soucek et al. 2026). Available evidence indicates that the very high toxicity of 6PPD-q is specific to this chemical, as other quinone degradants have not been shown to cause effects in salmonid species at similar concentrations (Montgomery et al. 2023; Nair et al. 2025).

Freshwater acute toxicity

The following are the lowest median effective concentration (EC50), median lethal concentration (LC50), and no observed effect concentration (NOEC) values reported for short-term exposures of freshwater model organisms across three trophic levels.

Acute endpoints for 6PPD were retrieved from the REACH dossier (ECHA CHEM n.d.-f), the SIDS report (OECD 2004) and the scientific literature (Prosser R. S. et al. 2017a) for this chemical. Acute endpoints for 6PPD-q were retrieved from the scientific literature (Liu J et al. 2024b; Prosser et al. 2023; Soucek et al. 2026). Data for both chemicals were also retrieved from the ECOTOX Knowledgebase (US EPA n.d.-b).

Acute endpoints for all other chemicals were retrieved from the respective REACH dossiers of the chemicals (ECHA CHEM n.d.-a; ECHA CHEM n.d.-b; ECHA CHEM n.d.-c; ECHA CHEM n.d.-d; ECHA CHEM n.d.-e; ECHA CHEM n.d.-g). Information for PaTaXPD was retrieved from the NICNAS assessment report for the chemical (NICNAS 2001).

Relevant endpoints for p-hydroquinone and aniline were retrieved from previous NICNAS and AICIS assessments (AICIS 2022b; NICNAS 2013). Endpoints for 4-aminophenol were retrieved from the OECD SIDS report for the chemical (OECD 2010).

Fish

Chemical	Endpoint	Method
6PPD	96 h LC50 = 0.028 mg/L	<i>Oryzias latipes</i> (Japanese medaka) Flow-through conditions, measured concentrations OECD TG 203
77PD	96 h LC50 = 0.06 mg/L	<i>Pimephales promelas</i> (fathead minnow) Flow-through conditions, measured concentrations OECD TG 204

Chemical	Endpoint	Method
44PD	96 h LC50 = 0.13 mg/L	<i>Pimephales promelas</i> (fathead minnow) Static conditions, nominal concentrations EPA660/3-75-009
7PPD	96 h LC50 = 0.3 mg/L	<i>Lepomis macrochirus</i> (bluegill) Static conditions, nominal concentrations EPA-660/3-75-009
IPPD	96 h LC50 = 0.41 mg/L	<i>Pimephales promelas</i> (fathead minnow) Flow-through conditions, measured concentrations EPA-660/3-75-009
PaTPD	96 h LC50 = 0.48 mg/L	<i>Oncorhynchus mykiss</i> (rainbow trout) Flow-through conditions, measured concentrations OECD TG 204
PaTaXPD	14 d LC50 = 0.35 mg/L	<i>Cyprinus carpio</i> (common carp) Flow-through conditions, measured concentrations OECD TG 204
6PPD-q	96 h LC50 = 0.000031 mg/L	<i>Oncorhynchus kisutch</i> (coho salmon) Flow-through conditions, measured concentrations (Soucek et al. 2026)
p-hydroquinone	96 h LC50 = 0.638 mg/L	<i>Oncorhynchus mykiss</i> (rainbow trout) Flow-through conditions OECD TG 203
4-aminophenol	96 h LC50 = 0.93 mg/L	<i>Oryzias latipes</i> (Japanese medaka) Flow-through conditions, measured concentrations OECD TG 203

Ecotoxicity endpoints are also available for the quinone degradants IPPD-q, CPPD-q and 77PD-q. All three have 96 hour LC50s > 0.05 mg/L for *Oncorhynchus mykiss* (rainbow trout) (Nair et al. 2025), indicating substantially reduced toxicity compared to 6PPD-q.

Invertebrates

Chemical	Endpoint	Method
6PPD	96 h LC50 = 0.25 mg/L	<i>Hyalella azteca</i> (amphipod) Static conditions, measured concentrations (Prosser et al. 2017a)
DPPD	48 h EC50 > 0.12 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Static conditions, nominal concentrations OECD TG 202
77PD	48 h EC50 = 0.2 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Static conditions, nominal concentrations EPA-660/3-75-009

Chemical	Endpoint	Method
7PPD	48 h EC50 = 0.2 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Static conditions, nominal concentrations EPA-660/3-75-009
44PD	48 h EC50 = 0.54 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Semi-static conditions, nominal concentrations OECD TG 202
PaTaXPD	48 h EC50 = 0.59 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Flow-through conditions, nominal concentrations OECD TG 202*
IPPD	48 h EC50 = 0.98 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Semi-static conditions, nominal concentrations EU method C.2
PaTPD	48 h EC50 > 1.1 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Flow-through conditions, measured concentrations OECD TG 202
6PPD-q	96 h LC50 > 0.23 mg/L	<i>Hexagenia sp.</i> (mayfly) Measured concentrations (Prosser et al. 2023)
4-aminophenol	48 h EC50 = 0.098 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Semi-static conditions, measured concentrations OECD TG 202
p-hydroquinone	48 h EC50 = 0.08 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Static conditions OECD TG 202
Aniline	48 h EC50 = 0.16 mg/L	<i>Daphnia magna</i> (water flea) Immobilisation Static conditions, measured concentrations EU method C.2

*incorrectly labelled as an OECD TG 115 study in the assessment report.

No invertebrate toxicity data were identified for quinone degradants other than 6PPD-q.

Algae

Chemical	Endpoint	Method
6PPD	96 h EC50 = 0.6 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions, nominal concentrations US EPA method
PaTPD	72 h EC50 > 0.079 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions, nominal concentrations OECD TG 201
DPPD	72 h EC50 = 0.099 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions, measured concentrations OECD TG 201
PaTaXPD	72 h EC50 = 0.11 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions, nominal concentrations OECD TG 201
44PD	72 h EC50 = 0.94 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions, measured concentrations OECD TG 201
IPPD	72 h EC50 = 26.5 mg/L	<i>Desmodesmus subspicatus</i> (green algae) Growth rate Static conditions, nominal concentrations EC method C.3
6PPD-q	72 h NOEC = 0.4 mg/L	<i>Chlorella vulgaris</i> (green algae) Growth rate Static conditions, nominal concentrations (Liu et al. 2024)
4-aminophenol	48 h EC50 = 0.15 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions, measured concentrations OECD TG 201
p-hydroquinone	48 h EC50 = 0.33 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions OECD TG 201

No algal or aquatic microorganism toxicity data were identified for quinone degradants other than 6PPD-q.

Marine acute toxicity

No marine acute toxicity data were available for the parent substituted *para*-phenylene diamines. Acute ecotoxicity data for 6PPD-q are available for planktonic embryos of two sea urchin species. The 48 hour growth EC50 values were 0.007 mg/L for *Paracentrous lividus* and 0.008 mg/L for *Arbacia lixula* (Calle et al. 2025).

Freshwater chronic toxicity

The following are the lowest no-observed effect concentration or equivalent effect concentration for 10% of organisms (EC10) values for chronic exposures of freshwater model organisms across three trophic levels.

Chronic endpoints for 6PPD were retrieved from the REACH dossier (ECHA CHEM n.d.-f) and the scientific literature (Liu J et al. 2024b; Shi et al. 2024). Chronic endpoints for 6PPD-q were retrieved from the scientific literature (Liu J et al. 2024b; Prosser et al. 2023; Roberts et al. 2025). Data for both chemicals were also retrieved from the ECOTOX Knowledge database (US EPA n.d.-b).

Chronic endpoints for all other substituted *para*-phenylenediamines are scarce and were retrieved from the REACH dossiers of the chemicals (ECHA CHEM n.d.-a; ECHA CHEM n.d.-b; ECHA CHEM n.d.-e; ECHA CHEM n.d.-g). Information for PaTaXPD was retrieved from the NICNAS assessment report for the chemical (NICNAS 2001).

Relevant endpoints for p-hydroquinone and aniline were retrieved from previous NICNAS and AICIS evaluation reports (AICIS 2022b; NICNAS 2013). Endpoints for 4-aminophenol were retrieved from the OECD SIDS report for the chemical (OECD 2010).

Fish

Chemical	Endpoint	Method
6PPD	41 d NOEC = 0.0385 mg/L	<i>Oryzias latipes</i> (Japanese medaka) Mortality Flow-through conditions, measured concentrations OECD TG 210
		<i>Pimephales promelas</i> (fathead minnow) Flow-through conditions, measured concentrations OECD TG 204
PaTPD	14 d NOEC = 0.14 mg/L	<i>Oncorhynchus mykiss</i> (rainbow trout) Mortality Flow-through conditions, measured concentrations OECD TG 204
		<i>Cyprinus carpio</i> (common carp) Mortality Flow-through conditions, nominal concentrations OECD TG 204
6PPD-q	45 d LC50 = 0.00039 mg/L	<i>Salvelinus namaycush</i> (lake trout) Semi-static conditions, measured concentrations (Roberts et al. 2025)
4-aminophenol	41 d LC50 = 0.064 mg/L	<i>Oryzias latipes</i> (Japanese medaka) Flow-through conditions, measured concentrations OECD TG 210

Chemical	Endpoint	Method
p-hydroquinone	32 d NOEC $\geq$ 0.066 mg/L	<i>Pimephales promelas</i> (fathead minnow) Reproduction Flow-through conditions, measured concentrations OECD TG 210
Aniline	32 d NOEC = 0.39 mg/L	<i>Pimephales promelas</i> (fathead minnow) Growth Flow-through conditions, measured concentrations OECD TG 210

Invertebrates

Chemical	Endpoint	Method
6PPD	21 d NOEC = 0.01 mg/L	<i>Daphnia pulex</i> (water flea) Mortality Semi-static conditions, nominal concentrations (Shi et al. 2024)
PaTPD	21 d NOEC = 0.016 mg/L	<i>Daphnia magna</i> (water flea) Mortality Semi-static conditions, measured concentrations OECD TG 211
44PD	21 d NOEC = 0.11 mg/L	<i>Daphnia magna</i> (water flea) Reproduction Semi-static conditions, measured concentrations OECD TG 211
6PPD-q	8 d NOEC = 0.011 mg/L	<i>Megaloniaias nervosa</i> (freshwater mussel) Mortality Semi-static conditions, measured concentrations (Prosser et al. 2023)
p-hydroquinone	21 d NOEC = 0.0057 mg/L	<i>Daphnia magna</i> (water flea) Reproduction Semi-static conditions OECD TG 211
Aniline	21 d NOEC = 0.004–0.024 mg/L	Various tests and effects
4-aminophenol	21 d NOEC = 0.055 mg/L	<i>Daphnia magna</i> (water flea) Reproduction Flow-through conditions, measured concentrations OECD TG 202 part 2

Algae

Chemical	Endpoint	Method
6PPD	10 d NOEC = 0.4 mg/L	<i>Chlorella vulgaris</i> (green algae) Growth rate Static conditions, nominal concentrations (Liu et al. 2024)
		<i>Selenastrum capricornutum</i> (green algae) Growth rate Static conditions, nominal concentrations OECD TG 201
PaTaXDP	72 h NOEC = 0.002 mg/L	<i>Selenastrum capricornutum</i> (green algae) Growth rate Static conditions, nominal concentrations OECD TG 201
PaTPD	72 h NOEC = 0.013 mg/L	<i>Selenastrum capricornutum</i> (green algae) Growth rate Static conditions, nominal concentrations OECD TG 201
DPPD	72 h EC10 = 0.049 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions, measured concentrations OECD TG 201
44PD	72 h NOEC = 0.096 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions, nominal concentrations OECD TG 201
p-hydroquinone	72 h NOEC = 0.019 mg/L	<i>Raphidocelis subcapitata</i> (green algae) Growth rate Static conditions OECD TG 201
4-aminophenol	72 h NOEC = 0.036 mg/L	<i>Pseudokirchneriella subcapitata</i> (green algae) Growth rate Static conditions, measured concentrations OECD TG 201
6PPD-q	10 d NOEC = 0.2 mg/L	<i>Chlorella vulgaris</i> (green algae) Growth rate Static conditions, nominal concentrations (Liu et al. 2024)

Marine chronic toxicity

Chronic ecotoxicity data are limited to 12-day NOEC values of 0.125 mg/L and 1 mg/L for the rotifer *Brachionus calyciflorus* exposed to 6PPD and 6PPD-q, respectively (Klauschies and Isanta-Navarro 2022).

Effects on terrestrial Life

Toxicity data for birds are only available for IPPD, with an estimated 11-day LD50 of 79.2 µg/egg in domestic hens (*Gallus gallus*), equivalent to 1.32 mg/kg (Korhonen et al. 1983).

Toxicity data for terrestrial plants are limited to 6PPD. No effects on the germination of pak choi (*Brassica rapa chinensis*) were observed at concentrations up to 0.1 mg/L (Liu J et al. 2024a). In addition, a 21-day growth no observed effect level of 0.25 mg/L was determined for clover seedlings grown under hydroponic conditions (Wang J-X et al. 2024).

Effects on sediment dwelling life

Toxicity data for sediment dwelling life are limited to 6PPD and 6PPD-q. The available data indicates that 6PPD and 6PPD-q may cause effects on sediment dwelling life.

A 28 day 10% lethal concentration (LC10) of 63 mg/kg dw was determined for the worm *Tubifex tubifex*. A 28-day LC10 of 68 mg/kg dw was determined for the amphipod *Hyaella azteca* (Prosser R. S. et al. 2017a).

Additionally, a 96 hour LC50 of 0.29 mg/L was determined for larvae of the mayfly *Neocloeon triangulifer* (Soucek et al. 2025), and a 28-day LC10 of 0.005 mg/L was determined for glochidia of the freshwater mussel *Lampsilis siliquoidea* (Prosser R. S. et al. 2017b). Both values were based on concentrations in the water phase.

Data for 6PPD-q include 96-hour NOEC values ranging from 0.05 to 0.23 mg/L in the water phase for larvae of the mayfly *Hexagenia* sp. (Prosser et al. 2023).

Endocrine effects/activity

No evidence of endocrine activity or adverse effects have been identified for the chemicals in this evaluation.

Predicted no-effect concentration (PNEC)

Predicted no-effect concentrations (PNECs) have been calculated for the water and sediment compartments to cover the range of chemicals and key degradants in this evaluation.

PNECs - Water

An aquatic PNEC of 4.5 µg/L was derived for the di-alkyl and alkyl aryl substituted *para*-phenylenediamines in this evaluation. An aquatic PNEC of 0.2 µg/L was derived for the di-aryl substituted *para*-phenylenediamines in this evaluation. An aquatic PNEC of 0.16 µg/L was derived for the worst-case transformation product of the chemicals in this evaluation.

The toxicity of 6PPD was considered to be representative of the worst-case scenario for the di-alkyl and alkyl aryl substituted *para*-phenylenediamines in this evaluation. 6PPD exhibited the lowest toxicity value out of the di-alkyl and alkyl aryl substituted *para*-phenylenediamines (see **Effects on Aquatic Life**). Additionally, 6PPD is the most extensively studied chemical in this evaluation with the most comprehensive ecotoxicity dataset.

As such, deriving a PNEC based on the information for 6PPD is expected to be protective of the effects of all di-alkyl and alkyl aryl substituted *para*-phenylenediamines in this evaluation.

Chronic ecotoxicity information for 6PPD were available for a broad range of species (14 aquatic species from 6 taxa). As such, a species sensitivity distribution (SSD) method was used to ensure that the calculated PNEC considered the extensive ecotoxicity information in a risk proportionate manner (see **Appendix**). The SSD method resulted in a 95% protective concentration (PC95) value of 4.5 µg/L for 6PPD. The PC95 value was

chosen as the aquatic PNEC for the di-alkyl and alkyl aryl substituted *para*-phenylene diamines in this evaluation, in line with typical considerations for slightly to moderately disturbed waterways across Australia (ANZG 2026).

The PNEC for di-aryl substituted *para*-phenylenediamines has been considered separately from the di-alkyl and alkyl aryl substituted *para*-phenylenediamines. The di-aryl substituted *para*-phenylenediamines exhibit much higher toxicity to algae and lower toxicity to fish than the other substituted *para*-phenylenediamines in this evaluation, including 6PPD. This suggests that separate consideration is warranted to ensure appropriate environmental protection. A PNEC of 0.2 µg/L for the di-aryl substituted *para*-phenylenediamines was derived from the lowest algae NOEC for PaTaXPD (growth rate NOEC = 2 µg/L; 0.002 mg/L) using an assessment factor of 10. This assessment factor was chosen as acute and chronic toxicity data was available for fish, invertebrates and algae for at least one di-aryl substituted *para*-phenylenediamines (EPHC n.d.).

Among the degradants of the chemicals assessed in this evaluation, 6PPD-q exhibited the highest toxicity, with toxicity to certain fish species at very low concentrations (see **Effects on Aquatic Life**). A wide range of ecotoxicity information is available for 6PPD-q, while information for the quinone degradants for the other chemicals in this evaluation is limited. As such, a PNEC has only been derived for the degradant 6PPD-q. The available ecotoxicity information for the other PPD-quinones indicates reduced toxicity compared to 6PPD-q, and so the PNEC for 6PPD-q is expected to be lower than any potential PNEC for the other PPD-quinones.

A species sensitivity distribution (SSD) method was used to estimate the 95% protective concentration (PC95) value of 0.16 µg/L for 6PPD-q (see **Appendix**). The PC95 value was chosen as the aquatic PNEC for the degradants of the chemicals in this evaluation, in line with typical considerations for slightly to moderately disturbed waterways across Australia (ANZG 2026).

It is noted that this PNEC value differs from the protection values for 6PPD-q derived by the US EPA and the British Columbia Ministry of Water, Land, and Resource Stewardship (BC MWLRS 2025; US EPA 2024b). These derivations result in protection values below the lowest observed endpoints for the most sensitive species (Coho Salmon, *Oncorhynchus kisutch*). This species and many of the species known to be the most sensitive to 6PPD-q are endemic to North America or Europe. Additionally, the very high toxicity of fish to 6PPD-q has been linked to differences in metabolic ability that are highly specific to certain fish species, rather than a broader toxic mode of action to all fish (Montgomery et al. 2023). While some salmonid species are sensitive to 6PPD-q at nanogram per litre concentrations, others are only affected by concentrations that are orders of magnitude higher (see **Appendix**). No 6PPD-q ecotoxicology information on native Australian fish, such as *Galaxiidae*, are available and the specific sensitivity of native Australian fish to 6PPD-q is unknown. As such, the 6PPD-q PNEC in this evaluation is intended to provide a reasonable level of protection for Australian aquatic life, without being overly conservative, in the absence of Australian specific toxicity data.

PNECs - Sediment

Insufficient information was available to estimate a sediment PNEC for various chemicals in this evaluation and relevant degradants. A sediment PNEC of 630 µg/kg dw was derived for 6PPD and a sediment PNEC of 174 µg/kg dw was derived for 6PPD-q.

Information on the toxicity of the chemicals or their degradants to sediment dwelling organisms is limited, with sediment toxicity information only available for 6PPD and 6PPD-q. Additionally, read-across to other substituted *para*-phenylenediamines and degradants is not suitable, due to the broad range of physicochemical properties, and indications of specific toxic modes of action to aquatic life. As such, sediment PNECs were derived only for 6PPD and for 6PPD-q.

A PNEC of 630 µg/kg dw for the 6PPD was derived from the chronic LC10 endpoint of 63 mg/kg dw for 6PPD in aquatic worms and an assessment factor of 100. A PNEC of 174 µg/kg dw for the 6PPD-q was derived from the chronic NOEC of 0.05 mg/L for 6PPD-q to mayfly larvae converted to sediment concentration according to equilibrium partitioning, and an assessment factor of 100. Assessment factors of 100 were appropriate for both PNECs as only one chronic value were available for both chemicals (EPHC n.d.).

Categorisation of environmental hazard

The categorisation of the environmental hazards of assessed chemicals according to domestic environmental hazard thresholds (DCCEEW 2022) is presented below:

Persistence

Not Persistent (Not P). Based on measured transformation half-lives for water, soil and sediment below the domestic thresholds for persistence, chemicals in this evaluation are categorised as Not Persistent.

Bioaccumulation

Bioaccumulative (B). Based on experimental bioconcentrations factors (BCFs) above 2,000 L/kg and log K_{OW} values greater than 4.2, DNPD and DTPD are categorised as Bioaccumulative.

Bioaccumulative (B). PaTPD is a UVCB substance known to contain DTPD. PaTaXPD is a UVCB substance known to contain DTPD, along with other tolyl and xylyl constituents (see **Chemical identity**). Based on experimental bioconcentrations factors (BCFs) above 2,000 L/kg and log K_{OW} values greater than 4.2 for DTPD, tolyl and xylyl substituted *para*-phenylenediamines, and xylyl and xylyl substituted *para*-phenylenediamines, PaTPD and PaTaXPD are categorised as Bioaccumulative

Not Bioaccumulative (Not B). Based experimental or estimated log K_{OW} values below 4.2 and experimental or estimated BCFs and BAFs below 2,000 L/kg, the remaining chemicals in this evaluation are categorised as Not Bioaccumulative.

Toxicity

Toxic (T). Based on experimental acute ecotoxicity values below 1 mg/L for a broad range of chemicals in this evaluation or read-across indicating that acute ecotoxicity values will be below 1 mg/L, all chemicals in this evaluation are categorised as Toxic.

GHS classification of environmental hazard

The chemicals in this evaluation satisfy the criteria for classification according to the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) for aquatic hazards

(UNECE, 2017). The classifications of the chemicals are based on available acute and chronic ecotoxicity information, as well as available degradability information and read-across principles.

Hydrolysis information, including tests in environmentally sampled water, is available for most chemicals in this evaluation. Chemicals were only considered to be rapidly degradable where the longest hydrolysis half-lives for the chemical were below 16 days, as per the guidance in the annexes to the GHS (UNECE 2017). DPPD and DTPD had maximum hydrolysis half-lives exceeding 16 days and were not considered to be rapidly degradable. DTPD is a constituent of PaTPD, and so PaTPD is also not considered to be rapidly degradable. All other chemicals were considered rapidly degradable.

Photolysis information from lab-based studies is available for some chemicals in this evaluation. Actual photochemical degradation is difficult to predict under environmental conditions due to the influence of factors such as water depth, turbidity, and suspended solids content (UNECE 2017). As such, photolysis information has not been considered in determining rapid degradation of substances.

Hazardous to the aquatic environment (acute / short term)

Based on experimental acute EC50 and LC50 values below 1 mg/L, the following chemicals satisfy the criteria for hazard category 'Aquatic Acute 1' with the hazard statement 'H400: Very toxic to aquatic life':

- DPPD (CAS RN 74-31-7)
- IPPD (CAS RN 101-72-4)
- 44PD (CAS RN 101-96-2)
- 6PPD (CAS RN 793-24-8)
- 7PPD (CAS RN 3081-01-4)
- 77PD (CAS RN 3081-14-9)
- PaTaXPD (CAS RN 68953-83-3)
- PaTPD (CAS RN 68953-84-4).

No experimental toxicity data are available for the other chemicals in this evaluation. These chemicals are structurally similar to at least one other chemical in this evaluation that has experimental information and are expected to have similar ecotoxicity (based on a read-across approach). Therefore, the following chemicals satisfy the criteria for hazard category 'Aquatic Acute 1' with the hazard statement 'H400: Very toxic to aquatic life':

- DNPD (CAS RN 93-46-9)
- CPPD (CAS RN 101-87-1)
- 4PPD (CAS RN 788-17-0)
- CCPD (CAS RN 4175-38-6)
- 33PD (CAS RN 4251-01-8)
- DTPD (CAS RN 27417-40-9).

Hazardous to the aquatic environment (chronic / long-term)

Based on experimental chronic NOEC values below or equal to 0.01 mg/L, the following chemicals satisfy the criteria for hazard category 'Aquatic Chronic 1' with the hazard statement 'H410: Very toxic to aquatic life with long lasting effects':

- 6PPD (CAS RN 793-24-8)

- PaTaXPD (CAS RN 68953-83-3).

Based on experimental chronic NOEC or EC10 values below or equal to 0.1 mg/L and non-rapid degradability, the following chemicals satisfy the criteria for hazard category 'Aquatic Chronic 1' with the hazard statement 'H410: Very toxic to aquatic life with long lasting effects':

- DPPD (CAS RN 74-31-7)
- PaTPD (CAS RN 68953-84-4).

No ecotoxicity information is available for DNPD (CAS RN 93-46-9) and DTPD (CAS RN 27417-40-9).

DTPD is structurally similar to DPPD and is also a substituent of PaTPD. Therefore, the ecotoxicity behaviour of DTPD will be similar to the behaviour of DPPD and PaTPD. DTPD satisfies the criteria for hazard category 'Aquatic Chronic 1' with the hazard statement 'H410: Very toxic to aquatic life with long lasting effects'.

DNPD is a di-aryl substituted *para*-phenylenediamine. All other di-aryl substituted *para*-phenylenediamines in this evaluation either have chronic NOEC value below 0.01 mg/L, or have non-rapid degradability with chronic NOEC or EC10 values below or equal to 0.1 mg/L. DNPD is expected to have ecotoxicity similar to the other di-aryl substituted *para*-phenylenediamines. Based on readacross from the other di-aryl substituted *para*-phenylenediamines, DNPD satisfies the criteria for hazard category 'Aquatic Chronic 1' with the hazard statement 'H410: Very toxic to aquatic life with long lasting effects'.

Based on rapid degradability and on experimental chronic NOEC or EC10 values above 0.01 mg/L but below or equal to 0.1 mg/L, the following chemicals satisfy the criteria for hazard category 'Aquatic Chronic 2' with the hazard statement 'H411: Toxic to aquatic life with long lasting effects':

- IPPD (CAS RN 101-72-4)
- 44PD (CAS RN 101-96-2).

Due to a lack of experimental ecotoxicity data and variability in chronic toxicity behaviour preventing reliable read-across, it is not possible to classify the following chemicals for long-term (chronic) toxicity:

- CPPD (CAS RN 101-87-1)
- 4PPD (CAS RN 788-17-0)
- 7PPD (CAS RN 3081-01-4)
- 77PD (CAS RN 3081-14-9)
- CCPD (CAS RN 4175-38-6)
- 33PD (CAS RN 4251-01-8).

Environmental risk characterisation

Based on the PEC and PNEC values determined above, the following Risk Quotients (RQ = PEC ÷ PNEC) have been calculated for the release of substituted *para*-phenylene diamines into environmental waters, the release of 6PPD-q into environmental waters, and releases of 6PPD and 6PPD-q into the aquatic environment resulting in partitioning to the sediment:

Compartment	Chemical	PEC	PNEC	RQ
Surface waters	Di-alkyl and, alkyl aryl substituted	2.7 µg/L	4.5 µg/L	0.6
Surface waters	Di-aryl substituted	0.16 µg/L	0.2 µg/L	0.8
Surface waters	6PPD-q	0.088 µg/L	0.16 µg/L	0.56
Sediment	6PPD	468 µg/kg	630 µg/kg	0.74
Sediment	6PPD-q	27 µg/kg	174 µg/kg	0.16

For surface waters, RQs less than 1 indicate that the chemicals in this evaluation are not expected to pose significant risks to aquatic organisms as environmental concentrations are below levels likely to cause harmful effects.

Current available monitoring information for 6PPD-q indicates that 6PPD-q concentrations are below levels likely to cause harmful effects in most species of aquatic life. However, Australian specific monitoring and ecotoxicity information on 6PPD-q is limited. Available information indicates that other PPD-quinones have lower ecotoxicity than 6PPD-q, while the use volumes of 6PPD are higher than the use volumes of all other *para*-phenylenediamines. As such, the RQs for the other PPD-quinone degradants are expected to be lower.

In sediments, RQs less than 1 for 6PPD and its degradant 6PPD-q indicate no significant risks to sediment dwelling organisms. The risks of other chemicals and degradants to sediment life cannot be characterised due to insufficient information.

Uncertainty

This evaluation was conducted based on a set of 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:

- Limited Australian monitoring data are available for parent chemicals and for key degradants including 6PPD-q. The data that are available for 6PPD-q covers a high exposure scenario for waterways in one Australian city (a storm event near a major highway in a major city). However, concentrations of 6PPD-q in urban waters in other major Australian cities are unknown. Additionally, no Australian monitoring information on any parent chemicals have been identified. Re-evaluation may be required if new information becomes available to indicate that concentrations in Australian waterways are higher than currently considered for the PECs.
- No toxicity information is available for Australian species of aquatic life for the chemicals in this evaluation or their degradants. Refinement of PNECs may be required if information becomes available to indicate that Australian species are unprotected by the derived PNEC values.
- The available bioaccumulation information is generally limited, with mixed results for some chemicals in this evaluation. Re-evaluation may be required if new information becomes available to indicate that the bioaccumulation of some chemicals in this evaluation has been underestimated.

Appendix

Species Sensitivity Distribution modelling for 6PPD and 6PPD-q

Ecotoxicity data for 6PPD and 6PPD-q were obtained from the ECOTOX Knowledgebase (US EPA n.d.-b).

Only data obtained from studies on the chemicals were selected. Data from formulations were excluded because the concentration of the chemicals could not be ascertained.

A single endpoint value was derived for each species in accordance with accepted methods for deriving species sensitivity distributions (Warne et al. 2025), with some deviations. Mortality endpoints were preferred because they were considered the most reliable and comparable across studies. For some species, the reported endpoints showed inconsistent relationships between effect concentrations and exposure durations. In these cases, geometric mean endpoint values were calculated using data from studies of different durations. For 6PPD, chronic endpoint values for some species were estimated by applying an acute-to-chronic ratio of 10 to acute endpoints. For 6PPD-q, no consistent difference in sensitivity was observed between acute and chronic endpoints in fish species. Therefore, both unadjusted acute data and chronic data were considered for deriving single-species endpoint values for 6PPD-q.

The dataset for 6PPD comprised 14 aquatic species from 6 taxa (fish, crustaceans, insects, bivalve molluscs, rotifers and algae). The dataset for 6PPD-q comprised 33 species from 8 taxa (fish, crustaceans, bivalve and gastropod molluscs, echinoderms, insects, rotifers and algae).

The SSDs were built using shinyssdtools v 0.5.3 (Dalgarno 2021), which fits six statistical models to the data and derives an averaged species sensitivity distribution from which protective threshold concentrations for the aquatic environment are calculated. The 95% protective concentration (PC95) values were calculated as 4.5 µg/L for 6PPD and 0.16 µg/L for 6PPD-q. The 90% protective concentration (PC90) values were calculated to be 7 µg/L for 6PPD and 0.43 µg/L for 6PPD-q.

Table 1. Endpoint values used for the Species Sensitivity Distribution of 6PPD. Endpoints are for survival unless specified otherwise.

Species name	Lifestage	Taxon	Endpoint	mg/L	References
<i>Lampsilis siliquoidea</i>	Juvenile	Bivalve	28 d LC10	0.005	(Prosser R. S. et al. 2017b)
<i>Hyalella azteca</i>	Juvenile	Crustacean	28 d LC10	0.006	(Prosser R. S. et al. 2017a)
<i>Daphnia pulex</i>	Neonate	Crustacean	21 d NOEC	0.010	(Shi et al. 2024)
<i>Gobiocypris rarus</i>	Juvenile	Fish	4 d LC50	0.019a	(Di et al. 2022)
<i>Pimephales promelas</i>	Juvenile	Fish	21 d LC10	0.020	(Prosser Ryan S. et al. 2017)
<i>Oncorhynchus kisutch</i>	Juvenile	Fish	1 d LC50	0.025a	(Tian et al. 2021)

Species name	Lifestage	Taxon	Endpoint	mg/L	References
<i>Noecloeon triangulifer</i>	Nymphs	Insect	4 d LC50	0.032a	(Soucek et al. 2025)
<i>Oryzias latipes</i>	Embryo	Fish	41 d NOEC	0.039	(MITE 2003)
<i>Daphnia magna</i>	Neonate	Crustacean	2 d NOEC 1 gen NOEC	0.051b	(Hiki et al. 2021; Yang L et al. 2025)
<i>Lampsilis fasciola</i>	Glochidia	Bivalve	2 d EC10	0.063	(Prosser R. S. et al. 2017b)
<i>Danio rerio</i>	Embryo	Fish	1-5 d NOEC	0.116b	(Hiki et al. 2021; Lv et al. 2025; Rao et al. 2024; Varshney et al. 2022; Zhang S-Y et al. 2023)
<i>Brachionus calyciflorus</i>	Culture	Rotifer	12 d NOEC growth rate	0.125	(Klauschies and Isanta-Navarro 2022)
<i>Chlorella vulgaris</i>	Culture	Algae	10 d NOEC growth rate	0.400	(Liu J et al. 2024b)
<i>Chlorella pyrenoidosa</i>	Culture	Algae	1-10 d NOEC chlorophyll A	1.590b	(Chen et al. 2024)

a: acute LC50/10

b: geometric mean of multiple endpoints

Table 2. Endpoint values used for the Species Sensitivity Distribution of 6PPD-quinone. Endpoints are for survival unless specified otherwise.

Species name	Lifestage	Taxon	Endpoint	mg/L	References
<i>Oncorhynchus kisutch</i>	Juvenile	Fish	1 d NOEC 1 d LOEC	0.00003b	(Greer et al. 2023a; Lo et al. 2023; Montgomery et al. 2023)
<i>Oncorhynchus clarkii clarkii</i>	Juvenile	fish	1 d LC10 4 d LC50	0.00008a	(Shankar et al. 2025)
<i>Salvelinus fontinalis</i>	Fry or fingerling	Fish	1 d LC10	0.00028	(Philibert et al. 2024)
<i>Salvelinus namaycush</i>	Juvenile	Fish	45 d LC50	0.00039c	(Roberts et al. 2025)
<i>Salvelinus leucomaenis</i>	Juvenile	Fish	4 d LC50	0.00064a	(Hiki and Yamamoto 2022)
<i>Oncorhynchus mykiss</i>	Juvenile	Fish	4 d LC50	0.0014a	(Brinkmann et al. 2022; Di et al. 2022; Nair et al. 2025)

Species name	Lifestage	Taxon	Endpoint	mg/L	References
<i>Arbacia lixula</i>	Embryo	Echinoderm	2 d NOEC, LOEC growth	0.0032b	(Calle et al. 2025)
<i>Paracentrotus lividus</i>	Embryo	Echinoderm	2 d NOEC, LOEC growth	0.0032b	(Calle et al. 2025)
<i>Micropterus nigricans</i>	Juvenile	Fish	2 d NOEC	0.0032	(Soucek et al. 2026)
<i>Micropterus dolomieu</i>	Juvenile	Fish	1 d NOEC	0.0035	(Soucek et al. 2026)
<i>Oncorhynchus masou</i>	Juvenile	Fish	1 d NOEC	0.0035	(Hiki and Yamamoto 2022)
<i>Salvelinus curilus</i>	Juvenile	Fish	1 d NOEC	0.0038	(Hiki and Yamamoto 2022)
<i>Pimephales promelas</i>	Adult	Fish	4 d NOEC growth	0.0097	(Anderson-Bain et al. 2023)
<i>Oncorhynchus clarkii lewisi</i>	Juvenile	Fish	1 d NOEC	0.010	(Montgomery et al. 2023)
<i>Daphnia pulex</i>	Neonate	Crustacean	21 d NOEC	0.010	(Shi et al. 2024)
<i>Oncorhynchus tshawytscha</i>	Juvenile	Fish	1 d NOEC 1 d LC10	0.011b	(Greer et al. 2023b; Lo et al. 2023; Montgomery et al. 2023)
<i>Planorbella pilsbryi</i>	Embryo	Gastropod	10 d NOEC	0.012	(Prosser et al. 2023)
<i>Salmo trutta</i>	Juvenile	Fish	2 d NOEC	0.012	(Foldvik et al. 2022)
<i>Oncorhynchus gorbusha</i>	Juvenile	Fish	2 d NOEC	0.013	(Foldvik et al. 2024)
<i>Megaloniaias nervosa</i>	Adult	Bivalve	8 d NOEC	0.014	(Prosser et al. 2023)
<i>Oryzias latipes</i>	Juvenile	Fish	4 d NOEC	0.034	(Hiki et al. 2021)
<i>Salmo salar</i>	Juvenile or alevin	Fish	1-2 d NOEC	0.035b	(Foldvik et al. 2022; Montgomery et al. 2023)
<i>Daphnia magna</i>	Neonate	Crustacean	21 d NOEC	0.042	(Prosser et al. 2023)
<i>Hyalella azteca</i>	Juvenile	Crustacean	4 d NOEC	0.043	(Hiki et al. 2021)
<i>Danio rerio</i>	Embryo	Fish	1-5 d NOEC	0.070b	(Hiki et al. 2021; Jankowski et al. 2025; Varshney et al. 2022; Zhang S-Y et al. 2023)

Species name	Lifestage	Taxon	Endpoint	mg/L	References
<i>Hexagenia sp.</i>	Larvae	Insect	4 d NOEC	0.11	(Prosser et al. 2023)
<i>Chlorella vulgaris</i>	Culture	Algae	10 d NOEC, LOEC growth rate	0.28b	(Liu J et al. 2024b)
<i>Sciaenops ocellatus</i>	Embryo	Fish	3 d NOEC	0.50	(Ackerly et al. 2024)
<i>Acartia tonsa</i>	Adult	Crustacean	2 d NOEC	1.00	(Calle et al. 2025)
<i>Brachionus calyciflorus</i>	Culture	Rotifer	12 d NOEC growth rate	1.00	(Klauschies and Isanta-Navarro 2022)
<i>Rhodomonas salina</i>	Culture	Algae	2 d NOEC abundance	1.00	(Calle et al. 2025)
<i>Sparus aurata</i>	Embryo	Fish	2 d NOEC	1.00	(Calle et al. 2025)
<i>Chlorella pyrenoidosa</i>	Culture	Algae	10 d NOEC abundance	2.00	(Chen et al. 2024)

a: acute LC50

b: geometric mean of multiple endpoints

c: chronic LC50

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