# Phenolic benzotriazoles: Environment tier II assessment

**30 June 2017**

## CAS Registry Numbers: 2440-22-4, 3147-76-0, 3846-71-7, 3896-11-5, 3864-99-1, 25973-55-1, 3147-75-9, 36437-37-3, 70321-86-7.



## Preface

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

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

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

Stage One of the implementation of this framework, which lasted four years from 1 July 2012, examined 3000 chemicals meeting characteristics identified by stakeholders as needing priority assessment. This included chemicals for which NICNAS already held exposure information, chemicals identified as a concern or for which regulatory action had been taken overseas, and chemicals detected in international studies analysing chemicals present in babies' umbilical cord blood.

Stage Two of IMAP began in July 2016. We are continuing to assess chemicals on the Inventory, including chemicals identified as a concern for which action has been taken overseas and chemicals that can be rapidly identified and assessed by using Stage One information. We are also continuing to publish information for chemicals on the Inventory that pose a low risk to

human health or the environment or both. This work provides efficiencies and enables us to identify higher risk chemicals requiring assessment.

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

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

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

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

## Disclaimer

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Acronyms & Abbreviations

## Grouping Rationale

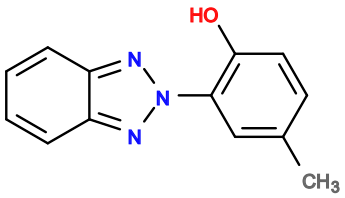
This Tier II assessment considers the environmental risks associated with industrial uses of nine related heterocyclic organic chemicals. The chemicals in this group all have a benzotriazole moiety attached to the *ortho*- position of a substituted phenol ring. This common structural feature provides the basis for the useful photochemical properties of this group of phenolic benzotriazoles.

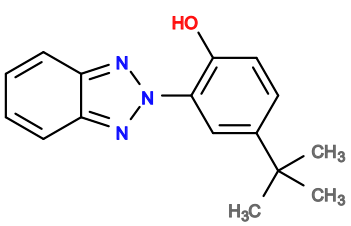
Phenolic benzotriazoles are able to absorb ultraviolet (UV) light without compromising their structural integrity. As a result, they are widely used as UV stabilisers in industrial applications such as automotive coatings and plastics to protect against photodegradation. They also have minor uses in cosmetics and personal care products (Danish EPA, 2015).

Some chemicals in this group have been identified as very persistent in the environment. There is also evidence that some are very bioaccumulative in aquatic organisms. Consequently, there are increasing concerns that some industrial uses of these chemicals may pose significant risks to the environment. This assessment will evaluate the currently available environmental hazard data for the chemicals in this group and will also seek to establish whether emissions of these chemicals to the Australian environment pose a concern.

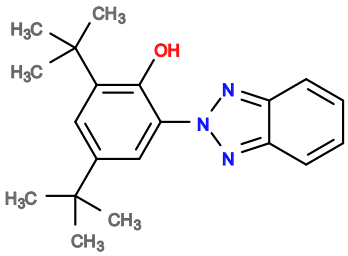
This assessment will also provide reference information for data-poor phenolic benzotriazoles listed on the Inventory which may also have applications as UV stabilisers in Australia. In addition, the hazard information compiled in this assessment provides reference information for analogous chemicals that may be formed through environmental degradation of more complex phenolic benzotriazoles that are listed on the Inventory.

## Chemical Identity

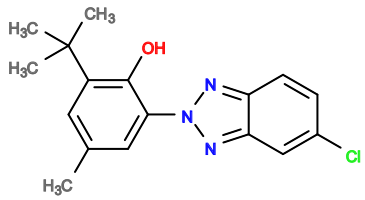
| | |
|---|---|
| CAS RN | 2440-22-4 |
| Chemical Name | Phenol, 2-(2*H*-benzotriazol-2-yl)-4-methyl- |
| Synonyms | UV-P<br>drometrizole |
| Structural Formula |  |
| Molecular Formula | $C_{13}H_{11}N_3O$ |
| Molecular Weight (g/mol) | 225.25 |
| SMILES | C12C(C=CC=C1)=NN(c1c(O)ccc(C)c1)N=2 |

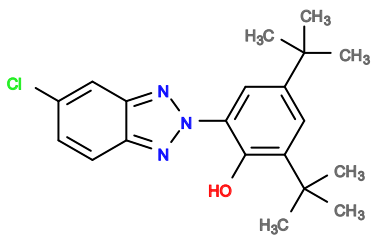
| | |
|---|---|
| CAS RN | 3147-76-0 |
| Chemical Name | Phenol, 2-(2*H*-benzotriazol-2-yl)-4-(1,1-dimethylethyl)- |
| Synonyms | UV-PS |
| Structural Formula |  |
| Molecular Formula | |

| | |
|---|---|
| | $C_{16}H_{17}N_3O$ |
| Molecular Weight (g/mol) | 267.33 |
| SMILES | C12C(C=CC=C1)=NN(c1c(O)ccc(C(C)(C)C)c1)N=2 |

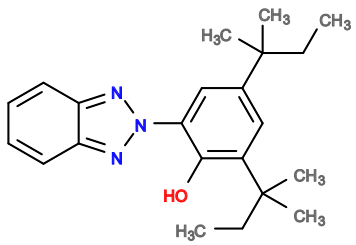
| | |
|---|---|
| CAS RN | 3846-71-7 |
| Chemical Name | Phenol, 2-(2*H*-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)- |
| Synonyms | UV-320 |
| Structural Formula |  |
| Molecular Formula | $C_{20}H_{25}N_3O$ |
| Molecular Weight (g/mol) | 323.43 |
| SMILES | C(C)(C)(C)c1c(O)c(N2N=C3C(C=CC=C3)=N2)cc(C(C)(C)C)c1 |

| | |
|---|---|
| CAS RN | 3896-11-5 |
| Chemical Name | Phenol, 2-(5-chloro-2*H*-benzotriazol-2-yl)-6-(1,1-dimethylethyl)-4-methyl- |
| Synonyms | UV-326<br>bumetrizole |

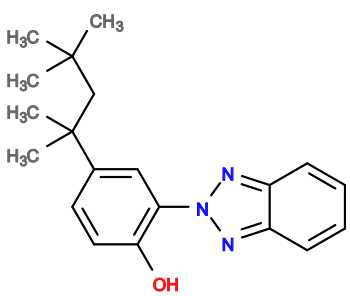
| | |
|---|---|
| Structural Formula |  |
| Molecular Formula | $C_{17}H_{18}ClN_3O$ |
| Molecular Weight (g/mol) | 315.80 |
| SMILES | C(C)(C)(C)c1c(O)c(N2N=C3C(C=C(Cl)C=C3)=N2)cc(C)c1 |

| | |
|---|---|
| CAS RN | 3864-99-1 |
| Chemical Name | Phenol, 2-(5-chloro-2*H*-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)- |
| Synonyms | UV-327 |
| Structural Formula |  |
| Molecular Formula | $C_{20}H_{24}ClN_3O$ |
| Molecular Weight (g/mol) | 357.88 |
| SMILES | C(C)(C)(C)c1c(O)c(N2N=C3C(C=C(Cl)C=C3)=N2)cc(C(C)(C)C)c1 |

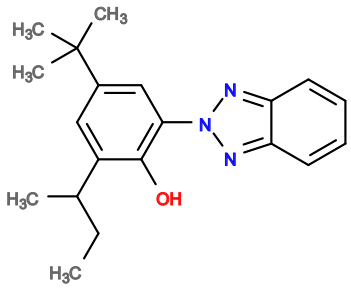
| | |
|---|---|
| CAS RN | 25973-55-1 |

| | |
|---|---|
| Chemical Name | Phenol, 2-(2*H*-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)- |
| Synonyms | UV-328<br>BDTP |
| Structural Formula |  |
| Molecular Formula | $C_{22}H_{29}N_3O$ |
| Molecular Weight (g/mol) | 351.49 |
| SMILES | C(C)(C)(c1c(O)c(N2N=C3C(C=CC=C3)=N2)cc(C(C)(C)CC)c1)CC |

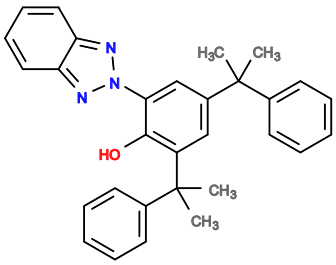
The following two chemicals in this group are structural isomers.

| | |
|---|---|
| CAS RN | 3147-75-9 |
| Chemical Name | Phenol, 2-(2*H*-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)- |
| Synonyms | UV-329<br>octrizole |
| Structural Formula |  |

| | |
|---|---|
| Molecular Formula | $C_{20}H_{25}N_3O$ |
| Molecular Weight (g/mol) | 323.43 |
| SMILES | C12C(C=CC=C1)=NN(c1c(O)ccc(C(C)(C)CC(C)(C)C)c1)N=2 |

| | |
|---|---|
| CAS RN | 36437-37-3 |
| Chemical Name | Phenol, 2-(2*H*-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)- |
| Synonyms | UV-350 |
| Structural Formula |  |
| Molecular Formula | $C_{20}H_{25}N_3O$ |
| Molecular Weight (g/mol) | 323.43 |
| SMILES | C12C(C=CC=C1)=NN(c1c(O)c(C(C)CC)cc(C(C)(C)C)c1)N=2 |

| | |
|---|---|
| CAS RN | 70321-86-7 |
| Chemical Name | Phenol, 2-(2*H*-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)- |
| Synonyms | UV-234 |

| | |
|---|---|
| Structural Formula |  |
| Molecular Formula | $C_{30}H_{29}N_3O$ |
| Molecular Weight (g/mol) | 447.57 |
| SMILES | c1(C(C)(C)c2c(O)c(N3N=C4C(C=CC=C4)=N3)cc(C(C)(C)c3ccccc3)c2)ccccc1 |

## Physical and Chemical Properties

Limited physical and chemical property data were identified for the chemicals in this group. The measured values available for UV-P are presented below (LMC, 2013):

| | |
|---|---|
| Physical Form | Solid |
| Melting Point | 133°C |
| Water Solubility | 0.17 mg/L |
| log $K_{ow}$ | 4.31 |

The chemicals in this group are expected to be solids at room temperature. Based on predicted p$K_a$ values (9.5–10.5) (LMC, 2013), most of the chemicals in this group will not be significantly ionised except under exceptional environmental conditions (pH > 9). They are not predicted to be significantly volatile.

The measured water solubility for the end-member of this group, UV-P, indicates that this chemical is only slightly soluble in water. All of the remaining chemicals in this group are more hydrophobic based on the range in estimated octanol-water partition coefficient ($K_{ow}$) values (log $K_{ow}$ = 4.36–7.67) (US EPA, 2008). Based on the typical trend of decreasing water solubility with increasing log $K_{ow}$, all of the remaining chemicals will have lower water solubility than UV-P and they can, therefore, all be considered as only very slightly soluble in water.

# Import, Manufacture and Use

## Australia

According to industry information, UV-P is used in industrial adhesives and UV-328 is used in industrial sealants in aftermarket automotive products.

No specific Australian use, import, or manufacturing information has been identified for the other chemicals in this group.

## International

Phenolic benzotriazoles are used internationally as UV stabilisers in a range of products. The chemicals protect against UV radiation and associated photodegradation (Danish EPA, 2015).

Approximately 50% of phenolic benzotriazoles produced globally are used in surface coatings (ECHA, 2014a). This group of chemicals is the most important type of UV stabilisers for automotive paints, particularly clearcoats, due to their resistance to photodegradation. They are also used in furniture treatments, such as varnishes, and adhesives and sealants (Danish EPA, 2015, ECHA, 2015a).

Approximately 40% of phenolic benzotriazoles produced globally are added to rubber products and plastics, including polyethylene terephthalate (PET) and polyvinyl chloride (PVC) (Danish EPA, 2015, ECHA, 2014a). These plastics are used to make a wide range of products, from disposable drink bottles through to toys for children and building materials (Danish EPA, 2015, ECHA, 2015a ).

The remaining production volume of phenolic benzotriazoles is expected to be used in other products, such as cosmetics and personal care products, where they can act as sunscreens and/or preservatives (Danish EPA, 2015, ECHA, 2014a). Two chemicals in this group (UV-P and UV-326) are permitted for use in cosmetic products in the EU (European Commission, 2013).

Some of the chemicals in this group are used in large volumes globally. For example, UV-P, UV-234, UV-328 and UV-329 are all identified as high production volume (HPV) chemicals by the OECD (OECD, 2015). Other chemicals in this group are also expected to be used in large volumes. For example, the annual introduction volume of UV-327 in Japan is approximately 550 tonnes (Kim, et al., 2011).

# Environmental Regulatory Status

## Australia

The industrial use of the chemicals in this group is not subject to any specific national environmental regulations.

## United Nations

None of the chemicals in this group are currently identified as a Persistent Organic Pollutant (UNEP, 2001), ozone depleting substance (UNEP, 1987), or hazardous substance for the purpose of international trade (UNEP & FAO, 1998).

## OECD

Four chemicals in this group (UV-P, UV-234, UV-328 and UV-329) are identified as HPV chemicals by the OECD, which indicates that more than 1000 tonnes of the chemical are produced per year in at least one member country. None of these

chemicals have been sponsored for assessment under the Cooperative Chemicals Assessment Programme (CoCAP) (OECD, 2015).

However, Japan has sponsored the assessment of three other chemicals in this group (UV-326, UV-327 and UV-350). The 28th Screening Information Dataset (SIDS) Initial Assessment Meeting (SIAM 28) found that UV-326 was a candidate for further work based on environmental concerns. The assessment of UV-327 and UV-350 is in the information gathering and data review stage (OECD, 2015).

The two remaining chemicals in this group have not been sponsored for assessment under CoCAP (OECD, 2015).

## Canada

All chemicals in this group (except UV-PS) were categorised during the Categorization of the Canadian Domestic Substances List (DSL) (Environment Canada, 2013a). Five chemicals (UV-234, UV-326, UV-328, UV-329 and UV-350) were categorised as not Persistent (P), but Bioaccumulative (B) and Inherently Toxic to the Environment ($iT_E$) (Environment Canada, 2013a). With the exception of UV-328, these chemicals are currently prioritised for further assessment (Environment Canada, 2013b). One chemical (UV-327) was categorised as P, but not B and not $iT_E$. The remaining chemicals (UV-P and UV-320) were categorised as not P and not B, and not $iT_E$ (UV-P) or $iT_E$ (UV-320) (Environment Canada, 2013a).

## European Union

Four chemicals in this group (UV-320, UV-327, UV-328 and UV-350) have been identified as Substances of Very High Concern (SVHC) under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation based on their very persistent and very bioaccumulative properties. For UV-320 and UV-328, potential toxicity in humans resulted in additional categorisation of these chemicals as Persistent, Bioaccumulative and Toxic (PBT) substances. All four chemicals are currently listed on the Candidate List of SVHCs for Authorisation (ECHA, 2016a).

Four additional chemicals in this group (UV-P, UV-234, UV-326 and UV-329) are currently subject to informal hazard assessments and risk management option analysis procedures under the SVHC Roadmap (ECHA, 2016b). If this work indicates that further action is needed, actions such as proposal for identification as a SVHC can be considered (ECHA, 2016c).

## United States of America

As part of the United States Environmental Protection Agency (US EPA) HPV Challenge Program, four chemicals in this group (UV-P, UV-234, UV-328 and UV-329) have been assessed. The chemicals were found to have high persistence and low to high bioaccumulation potential (US EPA, 2009).

## Japan

One chemical in this group (UV-320) has been identified as a Class I Specified Substance under the *Act on the Evaluation of Chemical Substances and Regulation of Their Manufacture, etc, 1973* (the Chemical Substances Control Law; CSCL). Class I Specified Substances are identified as persistent, highly bioaccumulative substances which pose a risk of long-term toxicity to humans or top predator animals (NITE, 2016). Permission is required to introduce these chemicals (METI, 2010).

Two additional chemicals in this group (UV-327 and UV-350) are identified as Monitoring Chemical Substances under the CSCL. These substances are persistent and highly bioaccumulative, with unclear long-term effects in humans or top predator animals (NITE, 2016). Introducers are required to report introduction volumes and use information (METI, 2010).

# Environmental Exposure

Domestic use data indicate two of the chemicals in this group are used in industrial adhesives and industrial sealants in the automotive aftermarket. Available international use data indicate that the chemicals in this group are used in a variety of

industrial applications, including in surface coatings (primarily automotive paint), in plastics and rubber. They may also be used in other products such as cosmetics and personal care products. A similar use pattern is expected in Australia.

Chemicals in this group may be released to sewer through routine cleaning of equipment used for the manufacture and application of surface coatings, or through the use of cosmetics and personal care products. Depending on the degradation and partitioning processes of chemicals in sewage treatment plants (STP), some fraction of the quantity of chemicals in wastewater entering STPs can be emitted to the air compartment, to river or oceans in treated effluent, or to soil through application of biosolids to agricultural land. Based on the moderate to high lipophilicity and low volatility of all chemicals in this group, and taking into account standard removal efficiencies, up to 85% of the total quantity of these chemicals entering a typical STP may be removed by adsorption to sludge, which may be applied to land as biosolids (Struijs, 1996). Hence, emissions of these chemicals to both environmental surface waters and soils are considered as part of this assessment.

The assumed uses of chemicals in this group in Australia and their release to sewers is supported by a recent analysis of wastewater entering a major municipal wastewater treatment plant in South Australia (Liu, et al., 2012). This study quantified the levels of UV-326 and UV-329 in influent waters and determined the partitioning and removal of these contaminants at various stages within this tertiary treatment plant.

# Environmental Fate

## Partitioning

The chemicals in this group are expected to primarily remain in their compartment of release, with movement from the water to the sediment compartment increasing with lipophilicity.

The chemicals in this group are very slightly soluble in water and very slightly volatile (ECHA, 2015a, LMC, 2013, OECD, 2009). Estimated Henry's Law constants for the group (< 6.6 x $10^{-8}$ Pa-$m^3$/mol) indicate very slight volatility from water and moist soil (US EPA, 2008). The log $K_{ow}$ values available for the chemicals in this group (ECHA, 2015a, LMC, 2013, OECD, 2009) indicate moderate to high lipophilicity, which suggests limited mobility in soil.

Calculations with a standard multimedia partitioning (fugacity) model assuming equal and continuous distributions to air, water and soil compartments (Level III approach) predict that the chemicals in this group will mainly partition to the soil and sediment compartments (in total, more than approximately 90%), with minor partitioning to the water compartment (less than approximately 10%) (US EPA, 2008). Chemicals in this group are expected to remain in the soil compartment if released solely to soil (US EPA, 2008). With sole release to the water compartment, the chemicals in this group are expected to partition between water and sediment. The partitioning to sediment increases with the lipophilicity of the chemical. For the most hydrophilic member of the group (UV-P), approximately 20% of the released volume is expected to partition to the sediment compartment. However, for the most lipophilic member of the group (UV-234), 98% is expected to partition to the sediment compartment (US EPA, 2008).

## Degradation

The chemicals in this group are expected to be persistent in the environment.

The core phenolic benzotriazole structure of chemicals in this group is expected to be resistant to abiotic degradation (ECHA, 2014a). This high abiotic stability is one of the primary functional characteristics required for the various industrial applications of these chemicals.

The biodegradation of the chemicals in this group is expected to proceed through either degradation of the benzotriazole moiety or degradation of the side chain in the *para*-position to the hydroxyl group on the phenol ring. Simulated biodegradation pathways for some phenolic benzotriazoles (e.g., UV-320) suggest that the bond between the benzotriazole and phenol rings is not cleaved during mineralisation of these chemicals (ECHA, 2014a).

A study conducted in accordance with OECD Test Guideline (TG) 301B demonstrates that UV-P, with the simplest *para*-substituent (a methyl group) and no other side chains, will be resistant to aerobic biodegradation under typical environmental conditions (2% biodegradation in 28 days) (LMC, 2013). As all other chemicals in this group have the same or more complex

side chains (with more highly branched side chains being more resistant to biodegradation), they are also expected to be resistant to biodegradation under typical environmental conditions. This is consistent with the results from ready biodegradation studies available for six further chemicals in this group (UV-320, UV-326, UV-328, UV-350, and UV-234; < 10% biodegradation in 28 days) (ECHA, 2015a, LMC, 2013).

Dissipation studies available for sediment and soil systems also suggest low biodegradation potential in these compartments for the chemicals in this group (ECHA, 2014a).

### Bioaccumulation

Most of the chemicals in this group are expected to be highly bioaccumulative.

The bioconcentration potential of discrete organic chemicals is generally related to the lipophilicity of a substance. Experimental bioconcentration factors (BCF) for two of the less lipophilic chemicals in this group (UV-P and UV-326) indicate moderate bioaccumulation potential. For UV-P, a BCF of 494 L/kg (normalised for 4% lipid content) was obtained for the fish *Cyprinus carpio* (common carp) after 56 days exposure at 1 mg/L; the test was conducted using flow-through conditions and solubilisers to maintain exposure concentrations (LMC, 2013). For UV-326, which has a predicted log $K_{ow}$ of 5.6 (US EPA, 2008), a maximum BCF of 895 L/kg was obtained for *C. carpio* after 70 days exposure at 0.005 mg/L (LMC, 2013). Experimental bioconcentration data were not available for UV-PS. However, this chemical is predicted to have lipophilicity that is intermediate between UV-P and UV-326 (i.e., log $K_{ow}$ = 4.36), and is, therefore, expected to have similar moderate bioconcentration potential in fish.

More lipophilic chemicals in this group have high to very high bioaccumulation potential. Experimental BCFs of 8180 L/kg, 8817 L/kg, 3681 L/kg and 34 391 L/kg have been determined for UV-320, UV-327, UV-328 and UV-350, respectively. All values were normalised to 5% lipid, and all studies were conducted according to OECD TG 305 using *C. carpio* (ECHA, 2014a, b, 2015b, c). Predicted log $K_{ow}$ values for these chemicals range from 6.27 to 7.25, with peak bioconcentration potential for UV-350 associated with a predicted log $K_{ow}$ of 6.31 (US EPA, 2008). No experimental BCF data were available for UV-329 or UV-234. However, with predicted log $K_{ow}$ values of 6.21 and 7.67, respectively, these chemicals are also expected to have a high bioconcentration potential in fish.

### Transport

The chemicals in this group are not expected to undergo long range transport.

The phenolic benzotriazoles in this group have low to very low water solubility, low volatility, and low mobility in soil. Based on these characteristics, transport in the environment through air or oceanic currents is expected to be limited. Instead, chemicals in this group are expected to accumulate in soils and sediments.

## Predicted Environmental Concentration (PEC)

A PEC for UV-P in river water of 0.33 micrograms per litre (µg/L) was estimated assuming typical removal efficiencies for the chemical in a secondary wastewater treatment plant.

Limited quantitative environmental monitoring data are available for the chemicals in this group. However, many have been detected in the environment. In Germany, UV-234, UV-320, UV-326, UV-327, UV-328, UV-329, and UV-350 have all been detected in river sediment and suspended particulate matter in the low nanograms per gram (ng/g) dry weight range (Wick, et al., 2016). A monitoring study undertaken by the Norwegian Environmental Protection Agency has also detected UV-234 in treated wastewater and landfill leachate, UV-327 and UV-329 in STP sludge, and UV-327 and UV-328 in sediment (Danish EPA, 2015).

A study of corrosion inhibitors and UV filters entering the Bolivar municipal wastewater treatment plant in Adelaide included UV-329 and UV-326 (Liu, et al., 2012). The maximum mean measured concentration of UV-329 in wastewater influent was 414 ± 261 nanograms per litre (ng/L), and 35 ± 8 ng/L for UV-326. The maximum mean measured concentrations in the secondary effluent were 98 ± 11 ng/L (UV-329) and 55 ± 14 ng/L (UV-326). Both chemicals were efficiently removed by the tertiary treatment process at this plant with no detectable residues present in the final tertiary treated effluent. The concentrations of

both chemicals in the biosolids produced at this plant were also measured. The mean measured concentration of UV-329 in biosolids was 27 ± 0.1 ng/g (or 27 µg/kg) and for UV-326 it was 88 ± 12 ng/g (or 88 µg/kg).

There is currently no domestic volume of use information available for any of the chemicals in this group. If a default annual introduction volume of 100 tonnes is assumed with 10% release to sewer then the average concentration of the chemicals in this group in the influent to an STP is estimated to be 8 500 ng/L (or 8.5 µg/L). Based on the available measured concentrations for the Bolivar plant, these estimated influent concentrations would be a significant overestimate. Hence, for the purposes of this assessment, the maximum mean measured concentration of UV-329 in the influent to the Bolivar plant (414 ng/L) is taken to be indicative of the concentrations of the chemicals in this group entering STPs in Australia.

Although substantial removal of the more lipophilic members of this group can be expected in STPs by adsorption to sludge, the more hydrophilic chemicals such as UV-P are less likely to be removed by partitioning processes. Based on standard removal efficiencies calculated assuming partitioning from water to sewage sludge (Struijs, 1996), 21% of the load of UV-P in wastewater influent would be expected to be removed to sludge and the remainder discharged in the effluent. According to this analysis, the concentration of UV-P in treated secondary effluent discharged to surface waters would be on the order of 330 ng/L (or 0.33 µg/L).

# Environmental Effects

# Effects on Aquatic Life

The results of most standard short- and long-term aquatic toxicity tests available for the chemicals in this group show that they have no toxic effects on aquatic life up to the limit of their respective solubilities in water. The chemicals in this group have very limited solubility in water, which may result in low bioavailability in the aquatic environment.

## Acute toxicity

Acute ecotoxicity studies for model organisms across three trophic levels were identified for five chemicals in this group (UV-P, UV-326, UV-328, UV-329, and UV-234) (ECHA, 2015a, LMC, 2013, OECD, 2009). The results of these studies showed that these very slightly soluble chemicals would not cause toxic effects at saturation levels. As these tests include results for the least lipophilic chemical in the group (UV-P) and the most lipophilic chemical (UV-234), they are expected to reliably represent acute ecotoxicity for the entire group.

## Chronic toxicity

The following no-observed effect-concentration (NOEC) value for the effects of UV-P on a model organism representing one trophic level was reported in the European Chemicals Authority Registered Substances Database (ECHA, 2015a):

| Taxon | Endpoint | Method |
|---|---|---|
| Invertebrates | 21 d NOEC = 0.013 mg/L | Experimental<br>*Daphnia magna* (Water flea)<br>OECD TG 211; semi-static<br>Measured concentrations<br>Reproductive toxicity and increased mortality observed |

Available chronic ecotoxicity data for other chemicals in this group (UV-326, UV-329, UV-328, and UV-234) indicate no effects at saturation levels in standard chronic ecotoxicity tests, although it is noted that no fish studies were identified (ECHA, 2015a, LMC, 2013).

Phenolic benzotriazoles have been found to cause activation of the aryl hydrocarbon receptor (AhR) pathway in exposed cells. This, coupled with the stability of the chemicals, suggests potential for chronic physiological effects of the type caused by dioxins (Nagayoshi, et al., 2015). Two chemicals in this group (UV-P and UV-326) have been found to cause activation of the AhR pathway in zebrafish (*Danio rerio*) embryos (Fent, et al., 2014). However, there is currently no evidence of organism level adverse effects resulting from this biochemical effect.

Fent et al. (2014) has studied the endocrine activity of phenolic benzotriazoles using yeast assays. They found that UV-P, UV-320, UV-326, UV-327, UV-328 and UV-329 do not have (o)estrogenic or androgenic activity. However, UV-P was found to have significant antiandrogenic activity (Fent, et al., 2014).

## Effects on Terrestrial Life

Chemicals in this group can cause toxic effects in terrestrial life.

No ecotoxicity studies on terrestrial life were located for the chemicals in this group. However, studies undertaken on terrestrial organisms to evaluate human toxicity potential were identified. Data from studies undertaken on UV-320 have found repeat oral dosage of rats at 0.5 milligrams per kilogram body weight per day (mg/kg bw/d) caused enlargement of liver cells (hepatocytes), with higher doses causing hepatocyte necrosis as well as kidney and spleen changes (ECHA, 2013). A rat repeat-dose study conducted using UV-350 also found a lowest-observed effect-level (LOEL) of 0.5 mg/kg bw/d (LMC, 2013). A similar study with UV-328 conducted on rats at higher dosages (> 5 mg/kg bw/d), found liver damage and discolouration (ECHA, 2013).

A LOEL of 30 mg/kg bw/d for rats is available for UV-P, with an increase in liver weight observed (LMC, 2013).

## Predicted No-Effect Concentration (PNEC)

Most of the chemicals in this group are persistent and bioaccumulative. These two hazard characteristics combined have the potential to result in a range of long term effects on organisms exposed to these chemicals which cannot be readily identified through standard ecotoxicity tests. For such chemicals, it is not currently possible to estimate a safe exposure concentration using standard extrapolation methods based on laboratory screening levels tests. Predicted no-effects concentrations have therefore not been derived for these chemicals.

For the remaining chemicals in this group, ecotoxicity information sufficient for the derivation of a PNEC is only available for one chemical. Results from the 21 d aquatic invertebrate test for UV-P were used to derive an aquatic PNEC. The PNEC for UV-P is calculated to be 0.13 µg/L, based on the 21 d NOEC of 0.013 mg/L and an assessment factor of 100. An assessment factor of 100 was selected for the PNEC derivation as there is only a single measured chronic ecotoxicity value available.

## Categorisation of Environmental Hazard

The categorisation of the environmental hazards of the chemicals in this group according to domestic environmental hazard thresholds is presented below (EPHC, 2009, NICNAS, 2013):

## Persistence

Persistent (P). Based on the results of ready biodegradability studies available for chemicals in this group, the resistance of these chemicals to abiotic degradation, and the high structural similarity of these substances, all chemicals in this group are categorised as Persistent.

## Bioaccumulation

### UV-320, UV-327, UV-328, UV-329, UV-350, and UV-234

Bioaccumulative (B). Based on measured BCF values in fish greater than 2000 L/kg and high log $K_{ow}$ values, all six of these chemicals are categorised as Bioaccumulative.

### All remaining chemicals

Not Bioaccumulative (Not B). Based on the comparatively lower lipophilicity of the remaining chemicals in this group, and measured BCF values available for UV-P and UV-326 that are less than 2000 L/kg, all remaining chemicals in this group are categorised as Not Bioaccumulative.

## Toxicity

### UV-P

Toxic (T). Based on a chronic aquatic invertebrate ecotoxicity value below 0.1 mg/L, UV-P is categorised as Toxic.

### All remaining chemicals

Uncertain (Uncertain T). There is currently insufficient available information to conclude whether the chemicals in this group also have chronic toxic effects, especially in higher aquatic trophic levels. However, there are concerns that they may have chronic toxicity given the high bioaccumulation potential of most of these chemicals and evidence that some can activate the AhR pathway in fish. The toxicity of these remaining chemicals is therefore categorised as Uncertain.

## Summary

Phenol, 2-(2*H*-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)- (UV-320); phenol, 2-(5-chloro-2*H*-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)- (UV-327); phenol, 2-(2*H*-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)- (UV-328); phenol, 2-(2*H*-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)- (UV-329); phenol, 2-(2*H*-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)- (UV-350); and phenol, 2-(2*H*-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)- (UV-234) are categorised as:

- P
- B
- Uncertain T

Phenol, 2-(2*H*-benzotriazol-2-yl)-4-methyl- (UV-P) is categorised as:

- P
- Not B
- T

Phenol, 2-(2*H*-benzotriazol-2-yl)-4-(1,1-dimethylethyl)- (UV-PS); and phenol, 2-(5-chloro-2*H*-benzotriazol-2-yl)-6-(1,1-dimethylethyl)-4-methyl- (UV-326):

- P
- Not B

- Uncertain T

## Risk Characterisation

Six chemicals in this group (UV-320, UV-327, UV-328, UV-329, UV-350, and UV-234) have been categorised as persistent and bioaccumulative substances. Chemicals which are persistent and bioaccumulative remain in the environment and accumulate in biota over an extended period of time, even if new emissions of the chemicals cease. These characteristics can result in very high internal concentrations in exposed organisms, which may cause long-term toxic effects that are not readily identified through standard testing protocols. Chemicals with these hazard characteristics are, therefore, considered to be of concern for the environment.

Two chemicals in this group (UV-PS and UV-326) have been categorised as persistent and not bioaccumulative, but with uncertain toxicity. These chemicals are not expected to have acute toxic effects on aquatic organisms. The potential risks arising from chronic exposure to these persistent chemicals in the aquatic environment cannot be characterised currently due to a lack of adequate long-term aquatic toxicity data. However, it should be noted that a recent finding that UV-326 can activate the AhR pathway in fish increases the level of concern for emissions of these chemicals to the aquatic environment.

The final chemical in this group, UV-P, is persistent and toxic. The below risk quotient (RQ = PEC ÷ PNEC) for the riverine compartment has been calculated based on the PEC and PNEC values determined for UV-P:

| PEC (µg/L) | PNEC (µg/L) | RQ |
|---|---|---|
| 0.33 | 0.13 | 2.54 |

An RQ greater than 1 indicates that the chemical may pose an unreasonable risk to the environment, as environmental concentrations may exceed levels that cause harmful effects. However, it should be noted that this calculation is subject to significant uncertainty due to uncertainties in the PEC value which is based on measured concentrations for UV-329 in the influent to a municipal wastewater treatment plant in Australia. If the PEC is based on the measured concentration of UV-326 in influent waters (0.01 µg/L) at a comparable sampling time, the RQ for riverine discharge is 0.08 which would indicate a generally low risk to the aquatic compartment.

Insufficient data are available to characterise the risks posed by the release of these chemicals to the soil and sediment compartments. However, it should be noted that the measured concentrations of UV-326 and UV-329 in the biosolids produced at the Bolivar plant in South Australia are very low (< 0.1 mg/kg), which suggests that there is a low risk from these chemicals to the soil compartment from application in biosolids.

## Key Findings

The chemicals in this group are used as UV stabilisers in a range of products, predominantly in automotive paints, plastics and rubber products, but also in personal care products and cosmetics. Global production volumes are significant, and many phenolic benzotriazole UV stabilisers have been detected in the environment. Two chemicals in this group (UV-P and UV-328) have been reported by industry to be in use in Australia. A further two chemicals (UV-326 and UV-329) are known to be in use in Australia based on an analysis of wastewater at a major wastewater treatment plant in South Australia.

All of the chemicals in this group are categorised as persistent (P). Six of the chemicals (UV-320, UV-327, UV-328, UV-329, UV-350, and UV-234) are also highly bioaccumulative substances and they are categorised as bioaccumulative (B).

The chemicals in this group have low water solubility and they do not cause acute toxic effects in aquatic life. However, one chemical (UV-P) has high chronic aquatic toxicity and this chemical is categorised as toxic (T). There are concerns regarding the potential chronic toxicity of other chemicals in this group based on their high bioaccumulation potential and a recent finding that UV-P and UV-326 activate the AhR pathway in fish. The toxicity of the remaining chemicals in this group has been categorised as Uncertain.

The chemicals in this group are not expected to be present in significant concentrations in the effluent from tertiary wastewater treatment plants. However, more significant concentrations are likely to be present in the effluents from secondary wastewater treatment plants. A marginal risk to surface freshwaters from UV-P in treated effluent released from a secondary wastewater treatment plants has been identified. However, the significance of this risk is uncertain.

The majority of the chemicals in this group have been identified as persistent and bioaccumulative substances which are of concern for the environment. Further assessment of these chemicals under the IMAP Framework may be required if information becomes available to indicate they are toxic, or if significant concentrations of these chemicals are identified either in biota or in surface waters in Australia.

## Recommendations

No further assessment is currently required.

## Environmental Hazard Classification

In addition to the categorisation of environmental hazards according to domestic environmental thresholds presented above, the classification of the environmental hazards of the chemicals in this group according to the third edition of the United Nations' Globally Harmonised System of Classification and Labelling of Chemicals (GHS) is presented below (UNECE, 2009).

Phenol, 2-(2*H*-benzotriazol-2-yl)-4-methyl- (UV-P):

| Hazard | GHS Classification (Code) | Hazard Statement |
|---|---|---|
| Acute Aquatic | Not classified | - |
| Chronic Aquatic | Category 1 (H410) | Very toxic to aquatic life with long lasting effects |

All remaining chemicals:

| Hazard | GHS Classification (Code) | Hazard Statement |
|---|---|---|
| Acute Aquatic | Not classified | - |
| Chronic Aquatic | Category 4 (H413) | May cause long lasting harmful effects to aquatic life |

All eight remaining chemicals in this group are poorly water soluble, are not rapidly degraded, and have a tendency to bioaccumulate. Hence, according to the GHS guidance on classification of aquatic hazards, the long-term aquatic hazard of all of these chemicals is classified as category Chronic 4 (i.e., the "safety net" classification).

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