

Cinnamic aldehydes: Environment tier II assessment

01 July 2016

CAS Registry Numbers: 104-55-2, 101-39-3, 7492-44-6, 122-40-7, 101-86-0.



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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 the industrial uses of the five cinnamic aldehydes:

2-Propenal, 3-phenyl- (cinnamaldehyde)
2-Propenal, 2-methyl-3-phenyl- (methyl cinnamaldehyde)
Hexanal, 2-(phenylmethylene)- (butyl cinnamaldehyde)
Heptanal, 2-(phenylmethylene)- (amyl cinnamaldehyde)
Octanal, 2-(phenylmethylene)- (hexyl cinnamaldehyde)

The chemicals in this group all have industrial applications as fragrances. Fragrance ingredients are ubiquitous components of numerous classes of formulated products including cosmetics, personal hygiene products, and various household and industrial cleaning agents. These product types are used in high volumes and are released into sewers nationwide as a normal part of their use pattern. Industrial uses of cinnamic aldehydes, therefore, have significant potential to result in environmental exposure through release of the chemicals in the treated effluents and biosolids produced by sewage treatment plants.

The five chemicals in this group have been assessed together because they are all simple alkyl-chain homologues of the α,β -unsaturated aldehyde, cinnamaldehyde. All five members of this group are categorised as reactive toxicants and they are all expected to have the same mode of toxic action. Aldehydes can demonstrate excess aquatic toxicity relative to unreactive narcotic toxicants through the formation of Schiff bases with proteins, and α,β -unsaturated aldehydes can also have excess toxicity through Michael-type addition to proteins (Dimitrov, et al., 2004)

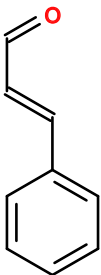
The Tier I assessment of cinnamaldehyde, amyl cinnamaldehyde and hexyl cinnamaldehyde indicated potential toxic hazard characteristics and unreasonable risks to the environment. This Tier II assessment includes further refinement of the risk

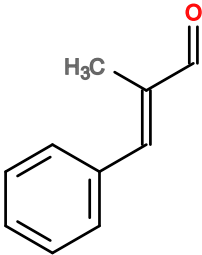
characterisation of these three chemicals and a more in-depth assessment of the available environmental hazard and exposure information. Although not identified under Stage One of the IMAP program, methyl cinnamaldehyde and butyl cinnamaldehyde have also been assessed as they are existing industrial chemicals listed on the Australian Inventory of Chemical Substances (the Inventory), and they are available for industrial uses, including as fragrance ingredients, in Australia.

Chemical Identity

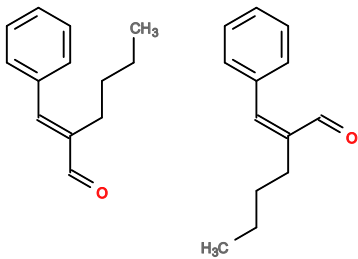
Most of the chemicals in this group including cinnamaldehyde and hexyl cinnamaldehyde are plant natural products that are present in some essential oils extracted from plants. For large scale applications such as in the flavouring and fragrance industries, these chemicals are synthesised. For example, technical cinnamaldehyde is synthesised by condensation of benzaldehyde (CAS RN 100-52-7) and acetaldehyde (CAS RN 75-07-0) (Little, 1989).

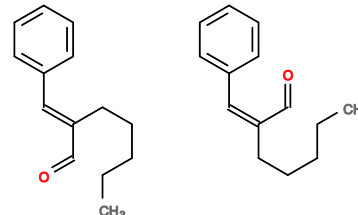
Cinnamaldehyde and methyl cinnamaldehyde used industrially consist predominantly of the *trans* isomer (EFSA, 2015; Klibanov and Giannousis, 1982; NTP, 2004). The relative proportions of the *trans* and *cis* isomers in technical butyl, amyl and hexyl cinnamaldehyde are unknown, and structures for both isomers have been provided in each case.

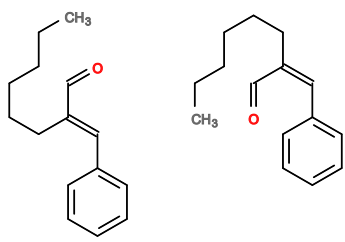
CAS RN	104-55-2
Chemical Name	2-Propenal, 3-phenyl-
Synonyms	cinnamaldehyde cinnamal
Structural Formula	
Molecular Formula	C ₉ H ₈ O
Molecular Weight (g/mol)	132.16
SMILES	<chem>c1ccccc1/C=C/C=O</chem>
CAS RN	101-39-3

Chemical Name	2-Propenal, 2-methyl-3-phenyl-
Synonyms	methyl cinnamaldehyde methyl cinnamal
Structural Formula	
Molecular Formula	C ₁₀ H ₁₀ O
Molecular Weight (g/mol)	146.19
SMILES	<chem>c1ccccc1/C=C(C)C=O</chem>

CAS RN	7492-44-6
Chemical Name	Hexanal, 2-(phenylmethylene)-
Synonyms	butyl cinnamaldehyde butyl cinnamal
Structural Formula	

	
Molecular Formula	C ₁₃ H ₁₆ O
Molecular Weight (g/mol)	188.27
SMILES	<chem>c1ccccc1/C=C\CCCCC=O</chem> <chem>c1ccccc1/C=C/CCCCC=O</chem>

CAS RN	122-40-7
Chemical Name	Heptanal, 2-(phenylmethylene)-
Synonyms	amyl cinnamaldehyde amyl cinnamal
Structural Formula	
Molecular Formula	C ₁₄ H ₁₈ O
Molecular Weight (g/mol)	202.29
SMILES	<chem>c1ccccc1/C=C\CCCCC=O</chem> <chem>c1ccccc1/C=C/CCCCC=O</chem>

CAS RN	101-86-0
Chemical Name	Octanal, 2-(phenylmethylene)-
Synonyms	hexyl cinnamaldehyde hexyl cinnamal
Structural Formula	
Molecular Formula	C ₁₅ H ₂₀ O
Molecular Weight (g/mol)	216.32
SMILES	<chem>c1ccccc1/C=C\CCCCC=O</chem> <chem>c1ccccc1/C=C/(CCCCC)C=O</chem>

Physical and Chemical Properties

Limited measured chemical property data are available for the substances in this group. Based on the available calculated and experimental values for key chemical properties, the water solubility and volatility of the chemicals in this group decreases as the carbon chain length of the homologue increases. Most substances in this group are expected to be at least moderately soluble in water and have moderate volatility (ECHA, 2016b; LMC, 2013; US EPA, 2008 ; 2016):

Chemical	cinnamaldehyde	hexyl cinnamaldehyde
Physical Form	liquid	solid
Melting Point	-7.5°C (exp.)	39.2°C (exp.)

Boiling Point	246°C (exp.)	175°C (exp., at 2000 Pa)
Vapour Pressure	3.85 Pa (exp.)	0.03 Pa (exp.)
Water Solubility	1420 mg/L (exp.)	5.44 mg/L (calc.)
Ionisable in the Environment	No	No
log K _{ow}	1.9 (exp.)	5.3 (exp.)

Import, Manufacture and Use

Australia

Cinnamaldehyde and hexyl cinnamaldehyde have reported commercial use in industrial cleaners. Cinnamaldehyde also has reported uses in automotive aftermarket products.

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

International

Available information indicates that the chemicals in this group are used as fragrances in a range of products internationally. All of the chemicals in this group are listed on the International Fragrance Association (IFRA) Transparency List, which identifies chemicals used as fragrances by member companies (IFRA, 2015). In addition, all are listed on the European Union (EU) Cosmetic Ingredients and Substances Database (CosIng) (European Commission, 2013). Formulated fragrances are used in cleaning and washing products, and most of the chemicals in the group (cinnamaldehyde, methyl cinnamaldehyde, amyl cinnamaldehyde, and hexyl cinnamaldehyde) are reported to be used internationally in household cleaning and washing products (Nordic Council of Ministers, 2016).

Cinnamaldehyde is also used in metal plating as a brightener and corrosion inhibitor (Sharma, 2011). Similarly, amyl cinnamaldehyde and hexyl cinnamaldehyde are reportedly used internationally in surface treatments, a category which includes substances used in metal plating (Nordic Council of Ministers, 2016).

Cinnamaldehyde is used widely as a food additive due to its flavouring properties, and as a pesticide and fungicide (National Library of Medicine, 2016). However, these applications are beyond the scope of this assessment.

Environmental Regulatory Status

Australia

The 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

Most of the chemicals in this group (cinnamaldehyde, methyl cinnamaldehyde, amyl cinnamaldehyde and hexyl cinnamaldehyde) have been identified as High Production Volume (HPV) chemicals by the OECD in 2004 and/or 2007. This identification indicates that more than 1000 tonnes of each chemical is produced per year in at least one member country of the OECD (OECD, 2004a).

Canada

All of the chemicals in this group were categorised as not Persistent (not P), not Bioaccumulative (not B), and not Inherently Toxic to the Environment (not iT_E) by Environment Canada during the Categorization of the Domestic Substances List (DSL), and they were not prioritised for further assessment (Environment Canada, 2013).

European Union

All of the chemicals in this group were pre-registered under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation. Cinnamaldehyde and methyl cinnamaldehyde have undergone the full registration process (ECHA, 2014; 2016b). Cinnamaldehyde is also listed under REACH as a biocidal active substance (ECHA, 2016a).

United States of America

All of the chemicals in this group are listed on the inventory of chemicals manufactured or processed in the USA, as published under the *Toxic Substances Control Act 1976* (TSCA) (US EPA, 2015).

Cinnamaldehyde, amyl cinnamaldehyde and hexyl cinnamaldehyde were listed as US High Production Volume (HPV) chemicals in 2010, indicating that at least 1 000 000 pounds (454 tonnes) of the chemicals are manufactured/imported into the United States of America (USA) per year (US EPA, 2013).

Environmental Exposure

Available international use data indicate that the chemicals in this group are used as components of synthetic fragrance additives which are incorporated into a wide variety of consumer products, including cosmetics and cleaning products (both household and commercial). The formulation of these products on the Australian market is assumed to be similar to those found internationally. Therefore, chemicals in this group are expected to be found in a range of household and commercial products available for use in Australia. Chemicals used in cosmetics and cleaning products are typically released to waste water as a normal part of their use in household and industrial applications, and release of the chemicals in this group to sewage treatment systems in Australia is, therefore, assumed.

International use data also indicate that a number of the chemicals in this group are used in industrial electroplating. Based on standard emission scenarios for industrial electroplating operations, some release of the chemicals used in electroplating is expected to occur in the rinse water and spent bath solutions that are disposed of as industrial waste water (Environment Australia, 1999; OECD, 2004b).

Depending on degradation and partitioning processes of chemicals in sewage treatment plants (STPs), some fraction of the quantity of chemicals in waste water entering STPs can be emitted to the air compartment, to rivers or oceans in treated effluent, or to soil by application of biosolids to agricultural land. Approximately 56% of the total quantity of the most lipophilic

member of this group (hexyl cinnamaldehyde) that enters a typical STP may be removed by adsorption to sludge, which may then be applied to land as biosolids (Struijs, 1996). Hence, the emissions of cinnamic aldehydes to both environmental surface waters and soils are considered as part of this assessment.

Environmental Fate

Partitioning

The chemicals in this group are expected to remain in soil, or partition to water and sediment, when released as a result of industrial uses.

The chemicals in this group are neutral organic chemicals that are slightly soluble to readily soluble in water, with water solubility decreasing with increasing carbon chain length of the homologue. The chemicals in this group are moderately volatile to volatile (LMC, 2013; US EPA, 2008) and have a range of calculated Henry's Law constants between 0.162 to 1.46 Pa-m³/mol (at 25°C) (US EPA, 2008). Based on these calculated Henry's Law constants, the chemicals in this group are considered moderately volatile from water and moist 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 compartment (between 67.6 and 74.7%) and the water compartment (between 23.9 and 31.8%), with minor partitioning to the sediment compartment (between 0.11 and 1.02%) (US EPA, 2008). The chemicals in this group are expected to remain in the soil compartment if released solely to soil (US EPA, 2008). However, assuming sole release to the water compartment, it is predicted that the chemicals in this group will partition predominantly to water (between 95.8 and 99.6%), with minor partitioning to sediment (between 0.34 and 4.08%) (US EPA, 2008).

Degradation

The chemicals in this group are not expected to be persistent in the environment and are expected to undergo rapid and ultimate biodegradation in water.

Cinnamaldehyde and methyl cinnamaldehyde have been found to be readily biodegradable in studies conducted in accordance with OECD Test Guideline (TG) 301B, undergoing 97 to 100% degradation in 28 days (ECHA, 2016b). Amyl cinnamaldehyde and hexyl cinnamaldehyde have also been found to be readily biodegradable in studies conducted in accordance with OECD TG 301F, undergoing 90 to 97% degradation in 28 days respectively (Api, et al., 2015; US EPA, 2016). No measured biodegradation data are available for butyl cinnamaldehyde, but rapid ultimate biodegradation is expected due to the structural similarity of the chemical to readily biodegradable homologues in this group.

Some partitioning to the air compartment of these chemicals is expected based on their volatility and their function as fragrances in industrial products. All of the chemicals in this group are predicted to undergo rapid photo-oxidation by hydroxyl radicals in the troposphere (half-life between 0.20 and 0.28 days) (US EPA, 2008).

Bioaccumulation

The chemicals in this group are not expected to bioaccumulate in aquatic organisms.

No experimental bioaccumulation data are available for the chemicals in this group. In the absence of experimental bioaccumulation data, log K_{OW} values can be used to provide an indication of bioaccumulation potential in aquatic organisms. The available log K_{OW} values for cinnamaldehyde, methyl cinnamaldehyde and butyl cinnamaldehyde (≤ 3.48) suggest low potential for bioaccumulation (ECHA, 2016b; US EPA, 2008). However, the available log K_{OW} values for amyl cinnamaldehyde and hexyl cinnamaldehyde (≥ 4.33) indicate a possible bioaccumulation hazard (US EPA, 2008).

However, these chemicals are expected to be susceptible to metabolism in fish which can significantly reduce the potential for bioconcentration. For example, calculations using a standard quantitative structure-bioconcentration relationship (QSBR) indicate that the bioconcentration factor (BCF) for hexyl cinnamaldehyde is 5733 L/kg for upper trophic level fish based solely on

the hydrophobicity of this chemical (US EPA, 2008). After including the estimated biotransformation half-life of hexyl cinnamaldehyde in fish (2.73 days), the BCF is 1000 L/kg, which is below the domestic categorisation threshold for a bioaccumulation hazard to aquatic life (2000 L/kg).

No evidence has been identified to indicate that these chemicals biomagnify through the aquatic food chain.

Transport

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

Cinnamic aldehydes are readily sorbed to soil, which is expected to limit their potential to undergo long-range transport in the environment. Although the substances are soluble in water and moderately volatile, cinnamic aldehydes have a short primary half life in water and are rapidly degraded in the atmosphere. No environmental monitoring data were identified to indicate their presence in remote areas.

Predicted Environmental Concentration (PEC)

No Australian environmental monitoring data were identified for these chemicals. Therefore, standard exposure modelling for the release of chemicals to surface water from STPs was used to estimate concentrations of each chemical in river water receiving treated effluents (EPHC, 2009; Struijs, 1996).

In accordance with the IMAP Framework, the annual maximum volume of each chemical in this group that is imported and/or manufactured in Australia for industrial uses is assumed to be 100 tonnes (NICNAS, 2013). Based on standard models for partitioning and biodegradation of chemicals in STPs, 87 to 92% of the chemicals in this group entering an STP are predicted to be removed from waste water. The PECs for the riverine compartment are calculated to be between 4.85 and 7.88 micrograms per litre ($\mu\text{g/L}$) for the chemicals in this group after taking into account substantial removal from waste water by sorption to sludge and biodegradation, and considering the assumed maximum annual introduction volume for each chemical.

Environmental Effects

Effects on Aquatic Life

The α,β -unsaturated aldehyde moiety in each chemical of this group is an electrophile which is known to undergo irreversible reactions with biological nucleophiles, including the reactive centres of proteins (Dimitrov, et al., 2004). These chemicals are therefore categorised as reactive toxicants which are expected to demonstrate excess toxicity compared with the toxic effects due to a reversible non-polar narcosis mode of action.

The excess toxicity effect is apparent in the acute toxicity data for the chemicals in this group. For example, in the case of cinnamaldehyde the calculated 96 hour LC50 for toxicity to fish by a non-polar narcosis mode of action is 158 mg/L (US EPA, 2012). This is a factor of 50 less toxic than the measured 96 hour LC50 for this chemical. Furthermore, all five chemicals in this group have comparable toxic potency despite a difference of more than three orders of magnitude in octanol-water partitioning coefficient (K_{ow}) between cinnamaldehyde and hexyl cinnamaldehyde. The weak correlation between the hydrophobicity of the toxicant and its acute toxicity has been noted previously for cinnamic aldehydes in this group and the effect is attributed to excess toxicity due to a Michael-type addition mode of action (Koleva, 2010).

Acute toxicity

The available data are measured median lethal concentration (LC50) and median effective concentration (EC50) values for (a) cinnamaldehyde, (b) methyl cinnamaldehyde, (d) amyl cinnamaldehyde, and (e) hexyl cinnamaldehyde, for model organisms across three trophic levels. The data were reported in registration dossiers for the chemicals under the EU REACH legislation or retrieved from databases included in the OECD QSAR Toolbox and the United States Environmental Protection Agency (US

EPA) High Production Volume Information System (ECHA, 2016b; LMC, 2013; US EPA, 2016). The LC50 and EC50 values have been reported in molar concentration units (micromoles per litre, $\mu\text{mol/L}$) in addition to standard mass concentration units in order to allow comparison of the toxic potency of the homologues in this group:

Taxon	Endpoint	Method
Fish	(a) 96 h LC50 = 3.1 mg/L (23.5 $\mu\text{mol/L}$)	Experimental <i>Danio rerio</i> (Zebrafish) EC Directive 92/69/EEC C.1 Acute Toxicity for Fish
	(e) 96 h LC50 = 1.7 mg/L (7.9 $\mu\text{mol/L}$)	Experimental <i>Pimephales promelas</i> (Fathead minnow) OECD TG 203
Invertebrates	(a) 48 h EC50 = 3.86 mg/L (29.2 $\mu\text{mol/L}$) (b) 48 h EC50 = 9.9 mg/L (67.7 $\mu\text{mol/L}$)	Experimental <i>Daphnia magna</i> (Water flea) OECD TG 202
	(d) 48 h EC50 = 1.1 mg/L (5.4 $\mu\text{mol/L}$)	Experimental <i>Daphnia magna</i> (Water flea) EC Directive 67/548/EWG C.2 Acute Toxicity for Daphnia
Algae	(a) 72 h EC50 = 4.07 mg/L (30.8 $\mu\text{mol/L}$) (b) 72 h EC50 = 14.8 mg/L (101.2 $\mu\text{mol/L}$) (d) 72 h EC50 = 1.88 mg/L (9.3 $\mu\text{mol/L}$)	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae) OECD TG 201

No ecotoxicity studies were identified for butyl cinnamaldehyde. However, based on the trends in toxicity for close homologues within this group and the assumed common mode of toxic action, butyl cinnamaldehyde is considered to have comparable acute toxicity to aquatic organisms to that demonstrated for other members of this group.

Chronic toxicity

The following no-observed-effect-concentration (NOEC) and measured effect concentration for ten percent of the population (EC10) values for model organisms in one trophic level for (a) cinnamaldehyde, (b) methyl cinnamaldehyde, and (d) amyl

cinnamaldehyde were reported in registration dossiers for the chemicals under the EU REACH legislation or retrieved from databases included in the US EPA High Production Volume Information System (ECHA, 2016b; US EPA, 2016):

Taxon	Endpoint	Method
Algae	(a) 72 h NOEC = 2.0 mg/L (15.2 µmol/L) (d) 72 h NOEC = 0.15 mg/L (0.7 µmol/L)	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae) OECD TG 201
	(b) 72 h EC10 = 6.1 mg/L (41.7 µmol/L)	Experimental <i>Desmodesmus subspicatus</i> (Green algae) OECD TG 201

Predicted No-Effect Concentration (PNEC)

The 48 h EC50 of 1.1 mg/L (5.4 µmol/L) for the acute toxic effects of amyl cinnamaldehyde on the aquatic invertebrate, *D. magna*, has been chosen as the pivotal aquatic endpoint for all members of this group. A PNEC of 11 µg/L for all members of this group has been derived after application of an assessment factor of 100 to the pivotal end-point.

An assessment factor of 100 was selected as there are considered to be sufficient aquatic toxicity data across all three trophic levels that are sufficiently representative of the acute effects of all five chemicals in this group. This analysis takes into account the common mode of action for acute effects of all five chemicals and the comparable potency of their effects in short term exposures to aquatic organisms.

Categorisation of Environmental Hazard

The categorisation of the environmental hazards of 2-propenal, 3-phenyl-; 2-propenal, 2-methyl-3-phenyl-; hexanal, 2-(phenylmethylene)-; heptanal, 2-(phenylmethylene)-; and octanal, 2-(phenylmethylene)- according to domestic environmental hazard thresholds is presented below (EPHC, 2009; NICNAS, 2013):

Persistence

Not Persistent (Not P). Based on the results of the ready biodegradability studies conducted on cinnamaldehyde, methyl cinnamaldehyde, amyl cinnamaldehyde and hexyl cinnamaldehyde, all chemicals in this group are categorised as Not Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on low log K_{OW} values and/or expected natural metabolism and regulation of internal concentrations, the chemicals in this group are categorised as Not Bioaccumulative.

Toxicity

Not Toxic (Not T). Based on measured acute toxicity endpoints of greater than 1 mg/L for the two end-members of this group, cinnamaldehyde and hexyl cinnamaldehyde, all chemicals in this group are categorised as Not Toxic.

Summary

2-Propenal, 2-methyl-3-phenyl-; 2-propenal, 2-methyl-3-phenyl-; hexanal, 2-(phenylmethylene)-; heptanal, 2-(phenylmethylene)-; and octanal, 2-(phenylmethylene)- are categorised as:

- Not P
- Not B
- Not T

Risk Characterisation

Risk quotients for the riverine compartment ($RQ = PEC \div PNEC$) for each of the chemicals in this group are presented below:

Chemical	PEC (µg/L)	PNEC (µg/L)	RQ
cinnamaldehyde	7.9	11	0.72
methyl cinnamaldehyde	7.9	11	0.72
butyl cinnamaldehyde	7.9	11	0.72
amyl cinnamaldehyde	6.6	11	0.60
hexyl cinnamaldehyde	4.9	11	0.45

The risk quotients for all chemicals are less than one, indicating that individually they do not pose an unreasonable risk to the environment, as environmental concentrations are not expected to exceed levels that cause harmful effects.

The individual risk quotients are in some cases only marginally less than one which indicates that the risks of these chemicals to the riverine compartment may be sensitive to relatively small increases in annual introduction volumes above the assumed current maximum of 100 tonnes. Moreover, the cumulative estimated concentration of the chemicals in this group is greater than the PNEC ($RQ \text{ (cumulative)} = 3.2$), which may indicate a potential risk to aquatic organisms if cumulative use volumes for industrial applications of these chemicals in Australia are of the order of 500 tonnes per annum or greater.

Insufficient data are available to characterise the risks posed by the release of these chemicals to the sediment and soil compartments. However, it is noted that all chemicals in this group are rapidly degradable and there is, therefore, a low risk that cinnamic aldehydes will accumulate in soils amended with biosolids.

Key Findings

The chemicals in this group are used internationally as fragrance compounds in a wide range of products, including cosmetics and cleaning products. They are also used in the metal plating industry as brighteners and corrosion inhibitors. A similar use pattern is assumed in Australia.

The chemicals in this group are readily biodegradable, have low bioaccumulation potential, and have moderate acute aquatic ecotoxicity. They can be released to domestic and industrial waste waters through their industrial uses as fragrances in cosmetic and cleaning products, and from their use as brighteners in metal plating. The estimated concentrations of individual chemicals in this group in river water after treatment of waste water in STPs are less than a common PNEC calculated for all members of this group. These estimated environmental concentrations do not include emissions resulting from non-industrial uses.

Further assessment of these chemicals under the IMAP Framework may be required if information becomes available to suggest that the cumulative concentration of these chemicals exceeds 11 µg/L in river water in Australia, or information becomes available that indicates that cumulative introduction volumes of chemicals in this group are of the order of 500 tonnes or greater per annum.

Chemicals in this group are not PBT substances according to domestic environmental hazard criteria.

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 2-propenal, 3-phenyl-; 2-propenal, 2-methyl-3-phenyl-; hexanal, 2-(phenylmethylene)-; heptanal, 2-(phenylmethylene)-; and octanal, 2-(phenylmethylene)- according to the third edition of the United Nations' Globally Harmonised System of Classification and Labelling of Chemicals (GHS) is presented below (UNECE, 2009):

Hazard	GHS Classification (Code)	Hazard Statement
Acute Aquatic	Category 2 (H401)	Toxic to aquatic life

The classification of the acute aquatic hazards posed by the chemicals in this group was performed based on the measured acute ecotoxicity data presented in this assessment (UNECE, 2007).

There are insufficient chronic toxicity data available to reliably classify the long-term aquatic hazards of the chemicals in this group.

References

Api AM, Belsito D, Bhatia S, Bruze M, Calow P, Dagli ML, Dekant W, Fryer AD, Kromidas L, La Cava S, Lalko JF, Lapczynski A, Liebler DC, Miyachi Y, Politano VT, Ritacco G, Salvito D, Shen J, Schultz TW, Sipes IG, Wall B and Wilcox DK (2015). RIFM fragrance ingredient safety assessment, alpha-amylcinnamaldehyde, CAS registry number 122-40-7. *Food Chem Toxicol*, **82 Suppl**, pp S20-8.

Dimitrov S, Koleva Y, Schultz TW, Walker JD and Mekenyan O (2004). Interspecies quantitative structure-activity relationship model for aldehydes: Aquatic toxicity. *Environmental Toxicology and Chemistry*, **23**(2), pp 463-470.

ECHA (2014). *Pre-registered substances*. European Chemicals Agency, Helsinki, Finland. Accessed 1 May 2014 at <http://echa.europa.eu>.

ECHA (2016a). *Biocidal Active Substances*. Helsinki, Finland. Accessed 1 April 2016 at <http://echa.europa.eu>.

ECHA (2016b). *Registered Substances Database*. European Chemicals Agency, Helsinki, Finland. Accessed 1 April 2016 at <http://echa.europa.eu>.

EFSA (2015). Scientific Opinion on the safety and efficacy of XTRACT® Evolution-B, Code X60-6930 (carvacrol, cinnamaldehyde and capsicum oleoresin), as a feed additive for chickens for fattening. *The EFSA Journal*, **13**(2), pp 4011.

Environment Australia (1999). *National Pollutant Inventory Emission Estimation Technique Manual for Electroplating and Anodising*. Environment Australia, Canberra, Australia. Accessed 6 February 2015 at <http://www.npi.gov.au>.

Environment Canada (2013). *Search Engine for the Results of DSL Categorization*. Environment Canada, Gatineau, Quebec, Canada. Accessed 21 November 2013 <http://www.ec.gc.ca>.

EPHC (2009). *Environmental Risk Assessment Guidance Manual for Industrial Chemicals*. The Department of the Environment, Canberra, Australia. Accessed 8 September 2015 at <http://www.scew.gov.au>.

European Commission (2013). *CosIng*. European Commission, Brussels, Belgium. Accessed 26 July 2013 at <http://ec.europa.eu>.

IFRA (2015). *Ingredients*. Geneva, Switzerland. Accessed 4 July 2015 at <http://www.ifraorg.org>.

Klibanov AM and Giannousis PP (1982). Geometric specificity of alcohol dehydrogenases and its potential for separation of trans and cis isomers of unsaturated aldehydes. *Proceedings of the National Academy of Sciences of the United States of America*, **79**, pp 3462-3465.

Koleva YK (2010). Prediction of α,β -unsaturated aldehydes from structure for acute aquatic toxicity. *Bulgaria Scientific Papers*, **37**, pp 79-84.

Little AD (1989). *Cinnamaldehyde. Draft report of Support for chemical nomination and selection process of the national toxicology program*. United States National Institutes of Health, Maryland, USA. Accessed 29 June 2016 at <https://ntp.niehs.nih.gov>.

LMC (2013). *The OECD QSAR Toolbox for Grouping Chemicals into Categories*, v 3.1. Laboratory of Mathematical Chemistry, University "Prof. Dr. Assen Zlatarov", Burgas, Bulgaria. Available at <http://oasis-lmc.org>.

National Library of Medicine (2016). *TOXNET*. National Library of Medicine, National Institute of Health, Washington, D.C. 2016 at <http://toxnet.nlm.nih.gov>.

NICNAS (2013). *Inventory Multi-tiered Assessment and Prioritisation (IMAP) Framework*. National Industrial Chemicals Notification and Assessment Scheme, Sydney, Australia. Accessed 12 November 2013 <http://www.nicnas.gov.au>.

Nordic Council of Ministers (2016). *Substances in Preparations in Nordic Countries (SPIN)*. Chemical Group, Nordic Council of Ministers, Copenhagen, Denmark. Accessed 1 March 2016 at <http://www.spin2000.net>.

NTP (2004). *Toxicology and Carcinogenesis Studies of Trans-Cinnamaldehyde (Microencapsulated) (Cas No. 14371-10-9) in F344/N Rats and B6C3F1 Mice (Feed Studies)*. United States Department of Health and Human Services National Toxicology Program. Accessed 29 June 2016 at <https://ntp.niehs.nih.gov>.

OECD (2004a). *The 2004 OECD List of High Production Volume Chemicals*. Organisation for Economic Cooperation and Development, Paris, France. Accessed 10 October 2014 at <http://www.oecd.org>.

OECD (2004b). *Emission Scenario Document on Metal Finishing*. Organisation for Economic Cooperation and Development, Paris, France. Accessed 6 February 2015 at <http://www.oecd-ilibrary.org>.

Sharma P (2011). Cinnamic acid derivatives: A new chapter of various pharmacological activities. *Journal of Chemical and Pharmaceutical Research*, **3**(2).

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

UNECE (2007). *Annex 9: Guidance on Hazards to the Aquatic Environment*. United Nations Economic Commission for Europe, Geneva, Switzerland. Accessed 20 October 2014 at <http://www.unece.org>.

UNECE (2009). *Globally Harmonised System of Classification and Labelling of Chemicals (GHS), 3rd Revised Edition*. United Nations Economic Commission for Europe, Geneva, Switzerland. Accessed 30 March 2016 at <http://www.unece.org>

UNEP (1987). *The Montreal Protocol on Substances that Deplete the Ozone Layer*. United Nations Environment Programme, Ozone Secretariat, Nairobi, Kenya. Accessed 12 March 2016 at <http://ozone.unep.org>.

UNEP (2001). *The Stockholm Convention on Persistent Organic Pollutants*. United Nations Environment Programme, Secretariat of the Stockholm Convention, Châtelaine, Switzerland. Accessed 31 March 2016 at <http://www.pops.int>.

UNEP & FAO (1998). *The Rotterdam Convention on the Prior Informed Consent procedure for Certain Hazardous Chemicals and Pesticides in International Trade*. United Nations Environment Programme and Food and Agriculture Organization of the United Nations, Châtelaine, Switzerland. Accessed 30 March 2016 at <http://www.pic.int>.

US EPA (2008). *Estimations Programs Interface (EPI) Suite™ for Microsoft Windows®, v 4.10*. United States Environmental Protection Agency, Washington DC, USA. Available at <https://www.epa.gov>.

US EPA (2012). *The ECOSAR (ECOLOGical Structure Activity Relationship) Class Program for Microsoft Windows®, v 1.11*. United States Environmental Protection Agency, Washington DC, USA. Available at <https://www.epa.gov>.

US EPA (2013). *High Production Volume (HPV) Challenge*. United States Environmental Protection Agency, Washington DC, USA. Accessed 11 June 2015 <http://www.epa.gov/hpv>.

US EPA (2015). *TSCA Chemical Substance Inventory*. United States Environmental Protection Agency, Washington DC, USA. Accessed 2 February 2015 at <http://www.epa.gov>.

US EPA (2016). *High Production Volume Information System (HPVIS)*. United States Environmental Protection Agency, Washington DC, USA. Accessed 1 April 2016 at <https://ofmext.epa.gov>.

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