Australian Government
Department of Health and Aged Care
Australian Industrial Chemicals Introduction Scheme

1,3-Dioxane, 2-(2,4-dimethyl-3-cyclohexen-1-yl)-5-methyl-5-(1-methylpropyl)- (Karanal)

Evaluation statement (EVA00171)

31 March 2025

Draft

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AICIS evaluation statement (EVA00171)

Subject of the evaluation

1,3-Dioxane, 2-(2,4-dimethyl-3-cyclohexen-1-yl)-5-methyl-5-(1-methylpropyl)- (Karanal)

Chemical in this evaluation

CAS name	CAS number
1,3-Dioxane, 2-(2,4-dimethyl-3-cyclohexen-1-yl)-5-methyl-5-(1-methylpropyl)-	117933-89-8

Reason for the evaluation

Evaluation Selection Analysis indicated a potential environmental risk.

Parameters of evaluation

This evaluation considers the environmental risks associated with the industrial uses of 2-(2,4-dimethyl-3-cyclohexen-1-yl)-5-methyl-5-(1-methylpropyl)-1,3-dioxane. The chemical is listed on the Australian Inventory of Industrial Chemicals (the Inventory).

The chemical has been assessed for its risks to the environment according to the following parameters:

- Australian introduction volumes at up to 1 tonne per year based on upper estimates provided by industry sources
- Industrial uses listed in the 'Summary of use' section
- Expected emission to sewage treatment plants (STPs) following consumer and commercial use.

In this evaluation the chemical will be referred to by its commercial name Karanal.

Summary of evaluation

Summary of introduction, use and end use

There is currently no specific information available about the end use of Karanal in Australia, but it is expected to be used as a fragrance ingredient in various products. Australian introduction volumes are estimated to be up to 175 kg/annum based on information from the International Fragrance Association (IFRA).

According to international use data, the chemical has functional use as a fragrance. As a result, the chemical may be used in the following end use categories:

- Personal care products (cosmetics)
- Cleaning and furniture care products

- Laundry and dishwashing products
- Air care products.

Available information indicates that the worldwide use of Karanal as a fragrance ingredient is declining due to restrictions in some jurisdictions.

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, the chemical is:

- Persistent (P)
- Bioaccumulative (B)
- Toxic (T)

Environmental hazard classification

The chemical satisfies the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) for environmental hazards as follows (UNECE 2017). This evaluation does not consider classification of physical and health hazards:

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

Summary of environmental risk

Based on the uses of the chemical, it is expected to be disposed to wastewater and released to the environment through sewage treatment plant (STP) effluents and biosolids.

The global use of Karanal is expected to be declining due to regulatory action in some jurisdictions and phase out by some industry groups. However, available use information suggests that the chemical is still in use in multiple jurisdictions, including Australia.

The chemical is persistent, bioaccumulative and toxic (PBT) according to domestic PBT criteria. Due to their persistence, PBT chemicals have the potential to become widely dispersed environmental contaminants. Once in the environment, persistent chemicals that are also highly bioaccumulative pose an increased risk of accumulating in exposed organisms, and of causing adverse effects. They may also biomagnify through the food chain resulting in very high internal concentrations, especially in top predators. As persistent and bioaccumulative chemicals accumulate and remain in environmental biota over long periods, it is difficult to predict their adverse effects. A safe environmental exposure level cannot be derived for PBT chemicals.

Since the chemical has PBT characteristics, there are potential significant long term risks to the environment from the manufacture, import and use of the chemical. Given these characteristics, there is a risk to the environment that requires management (see **Proposed means for managing risks**).

Karanal is an *unknown or variable composition, complex reaction products or biological materials* (UVCB) substance composed of stereoisomers of the main structure and a positional isomer. The PBT characteristics of the chemical and; therefore, the risk to the environment, extend to any of the specific stereoisomers of Karanal and its positional isomer, and any mixtures thereof.

Proposed means for managing risk

Environment

Recommendation to Department of Climate Change, Energy, the Environment and Water (DCCEEW)

It is recommended that the chemical be scheduled under the Industrial Chemicals Environmental Management (Register) Act 2021 (ICEMR Act), with application of appropriate risk management measures to minimise further release to the environment from its introduction and use:

In making the scheduling decision consideration should be given to the following:

- The chemical is persistent, bioaccumulative and toxic (PBT) according to domestic PBT criteria. A safe environmental exposure level cannot be derived for PBT chemicals.
- The chemical has known or potential use in products and end uses as listed in the 'Summary of introduction, use and end use' section.
- The global use of Karanal is expected to be declining due to regulatory action in some jurisdictions and phase out by some industry groups. However, available use information suggests that the chemical is still in use in multiple jurisdictions, including Australia.
- Karanal is UVCB substance composed of stereoisomers of the main structure and a positional isomer impurity. The PBT characteristics of the chemical and; therefore, the risk to the environment, extend to any of the specific stereoisomers of Karanal and its positional isomer, and any mixtures.
    - Regulatory action in Europe applies to 5-sec-butyl-2-(2,4-dimethylcyclohex-3-en-1-yl)-5-methyl-1,3-dioxane [1], 5-sec-butyl-2-(4,6-dimethylcyclohex-3-en-1-yl)-5-methyl-1,3-dioxane [2] any of the individual stereoisomers of [1] and [2] or any combination.

Conclusions

The Executive Director proposes to be satisfied that the identified risks to 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

Rationale

This evaluation considers the environmental risks associated with the industrial uses of 2-(2,4-dimethyl-3-cyclohexen-1-yl)-5-methyl-5-(1-methylpropyl)-1,3-dioxane (CAS number 117933-89-8), also referred to as the 2,4-isomer). The chemical is a UVCB comprised of stereoisomers (see **Chemical identity).**

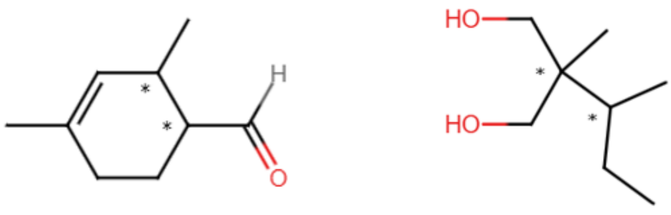
The chemical is often referred to by the commercial name Karanal which is comprised of the 2,4-isomer and the 4,6-positional isomer as an impurity.

The test studies used in this evaluation were drawn from REACH dossiers for the chemical and reaction products comprised of the 2,4- and 4,6-isomers (REACH n.d.-a; REACH n.d.-b; REACH n.d.-c) and an ECHA Substances of Very High Concern (SVHC) report on the chemical, the 4,6-positional isomer and any of their individual stereoisomers or any combination (ECHA 2015). The main source of information for this evaluation is the publicly available SVHC assessment, which is based on full study reports available to ECHA. Where information on the test substance has not been provided, it is assumed that it is on the main commercial form Karanal.

The Evaluation Selection Analysis (ESA) of Karanal indicated a need to assess the scale of use in Australia, as current industrial uses were unknown. The ESA highlighted potential persistent, bioaccumulative and toxic (PBT) hazard characteristics.

Chemical identity

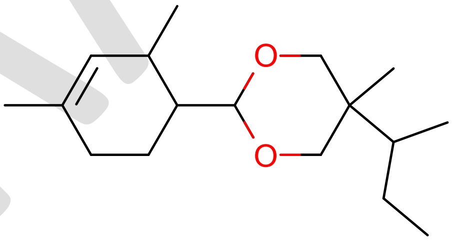
The chemical is an organic compound not found in nature and is a UVCB substance. The chemical structure is characterised by a methyl substituted cyclohexene ring that is connected to an alkyl substituted 1,3-dioxane moiety. The chemical is synthesised through acetalisation of chiral precursors (**Figure 1**) to produce 2,5-substituted 1,3-dioxane rings (ScenTree n.d.), which may exist as *cis* or *trans* stereoisomers. As a result, up to 16 stereoisomers may theoretically exist for the chemical (Cheng et al. 2009). The CAS name associated with CAS number 117933-89-8 does not specify the stereochemistry of the chemical. Therefore, the substance is assumed to be a UVCB comprised of stereoisomers.



CAS RN 68039-49-6   CAS RN 813-60-5

Figure 1. Structural formulae of Karanal precursors: 2,4-dimethyl-3-cyclohexene-1-carboxaldehyde (CAS number 68039-49-6) and 2-methyl-2-(1-methylpropyl)-1,3-propanediol (CAS number 813-60-5). Asterisks indicate chiral centres.

The chemical is often referred to by the commercial name Karanal. Available chemical identity information indicates that commercial samples of Karanal may include the chemical as well as the 4,6-isomer (CAS number 1781250-06-3, see chemical identity information below) (ECHA n.d.-c). In the 4,6-isomer the double bond is in a different position in the cyclohexene ring. Similarly to the 2,4-isomer, the 4,6-isomer may also be a UVCB comprised of stereoisomers. No distinction of isomers is made in perfumery (ScenTree n.d.).

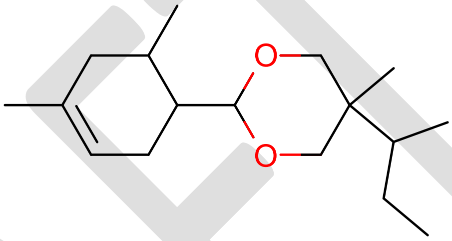
CAS number	117933-89-8
CAS name	1,3-Dioxane, 2-(2,4-dimethyl-3-cyclohexen-1-yl)-5-methyl-5-(1-methylpropyl)-
Molecular formula	$C_{17}H_{30}O_2$
Associated names	2-(2,4-Dimethylcyclohex-3-ene-1-yl)-5-methyl-5-(1-methylpropyl)-1,3-dioxane 2-Dimethylcyclohexenyl-5-methyl-5-methylpropyl-1,3-dioxane 5-(*sec*-Butyl)-2-(2,4-dimethylcyclohex-3-en-1-yl)-5-methyl-1,3-dioxane Karanal
Molecular weight (g/mol)	266.42
SMILES (canonical)	O1CC(C)(COC1C2CCC(=CC2C)C)C(C)CC
Structural formula	

Additional chemical identity information

The stereochemistry is not specified. The chemical is assumed to be a UVCB consisting of stereoisomers.

Related chemical

The 4,6-isomer below may be present in commercial samples of Karanal:

CAS number	1781250-06-3
CAS name	1,3-Dioxane, 2-(4,6-dimethyl-3-cyclohexen-1-yl)-5-methyl-5-(1-methylpropyl)-
Molecular formula	$C_{17}H_{30}O_2$
Associated names	2-(4,6-Dimethylcyclohex-3-ene-1-yl)-5-methyl-5-(1-methylpropyl)-1,3-dioxane 5-(sec-butyl)-2-(4,6-dimethylcyclohex-3-en-1-yl)-5-methyl-1,3-dioxane
Molecular weight (g/mol)	266.42
SMILES (canonical)	O1CC(C)(COC1C2CC=C(C)CC2C)C(C)CC
Structural formula	

Additional chemical identity information

The stereochemistry is not specified. The chemical is assumed to be a UVCB consisting of stereoisomers.

Relevant physical and chemical properties

Measured physical and chemical property data were retrieved from registration dossiers submitted under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation in the European Union (EU) and from the ECHA SVHC dossier for the substance (ECHA n.d.-c; REACH n.d.-b; REACH n.d.-c). The Henry's Law Constant value was calculated from the measured water solubility and vapour pressure values (US EPA 2017):

Physical form	liquid
Melting point	< -50°C (exp.)
Boiling point	> 250°C (exp.)
Vapour pressure	0.09 Pa (exp.)
Water solubility	0.61 mg/L (exp.)
Henry's law constant	39.3 Pa·m^3/mol (calc.)

Ionisable in the environment?	No
log K_{ow}	> 6.5 (exp.)

The chemical is a moderately volatile organic chemical with a slight solubility in water based on measured physicochemical properties.

Introduction and use

Australia

A voluntary call for information from industry identified that Karanal is used as a fragrance ingredient in Australia at low concentrations. The Australian use volume of Karanal in 2019 was estimated to be less than 350 kg/year based on data collected in the Asia-Pacific region by the International Fragrance Association (IFRA). Updated information from 2023 shows a decline in the use of the chemical, with an estimated annual volume of less than 175 kg for Australia. No specific Australian end use information has been identified.

International

Available information indicates that Karanal is used as a fragrance ingredient. The total reported international use volume for Karanal is up to 11 tonnes per annum.

The chemical is listed as a perfuming ingredient in the CosIng database (EC n.d.) and the estimated use volume in Europe is 1–10 tonnes per annum (REACH n.d.-b; REACH n.d.-c). Use of the substance has been prohibited in the European Economic Area (EEA) since 27 August 2023 (ECHA n.d.-b) and is; therefore, expected to be in decline. However, the chemical may still be available in other parts of the world. The chemical is on the IFRA Transparency List (IFRA n.d.; ScenTree n.d.). It is listed as ‘active’ on the US EPA Chemical Substance Inventory (US EPA 2024), which indicates that it has recently been manufactured, imported or processed by industry in the USA, but no use volume information is available (US EPA 2020). The chemical is a listed ingredient in 15 products sold on the US market, excluding reformulated or discontinued products (Johnson et al. 2023). The use volume for Canada is 0–1 tonne per year (OECD n.d.).

The chemical has reported end uses in polishes and waxes, washing and cleaning products and air care products, and in personal care products such as skin care, bath, shaving and hair care products (EC n.d.; Johnson et al. 2023; REACH n.d.-a; REACH n.d.-c). Karanal is listed as an ingredient in perfumes, some of which appear to have been discontinued or reformulated (Scentspiracy n.d.; Wikiparfum n.d.).

Recent volume information indicates that the use of Karanal is declining (Berbez 2016).

Existing Australian regulatory controls

Environment

The industrial use of the chemical is not subject to any specific national environmental regulations.

International regulatory status

United Nations

The chemical is not currently identified as a Persistent Organic Pollutant (POP) (UNEP 2001), ozone depleting substance (UNEP 1987), or hazardous substance for the purpose of international trade (UNEP & FAO 1998).

European Union

The chemical has been identified as a Substance of Very High Concern (SVHC) under the REACH legislation, due to very persistent and very bioaccumulative (vPvB) properties. The substance was included in REACH Annex XIV (Authorisation List) in 2020 and use of the chemical has been prohibited since 27 August 2023 (ECHA n.d.-b). No authorisation has been granted for the use of this chemical. The restrictions cover 5-sec-butyl-2-(2,4-dimethylcyclohex-3-en-1-yl)-5-methyl-1,3-dioxane [1], 5-sec-butyl-2-(4,6-dimethylcyclohex-3-en-1-yl)-5-methyl-1,3-dioxane [2] any of the individual stereoisomers of [1] and [2] or any combination.

Environmental exposure

Karanal is a synthetic compound that may be found as a fragrance ingredient in personal care, cleaning, laundry and air care products available for use in Australia. Products on the Australian market are assumed to be similar to those available internationally.

Chemicals used in personal care and cleaning products are typically released to wastewater as a normal part of their uses. Some fraction of the quantity of chemicals in wastewater entering STPs can also be emitted to the air compartment through volatilisation, to rivers or oceans in treated effluent, or to soil through application of biosolids to agricultural land (Struijs 1996). Chemicals used in air care products are emitted to the air compartment. The emissions of Karanal to environmental surface waters, soil and air are considered as part of this evaluation.

Available information indicates that Karanal is not used in large quantities. The chemical has recently been banned from use in Europe but may be found in products available in other parts of the world. No domestic or international monitoring data are available.

Environmental fate

Partitioning

Karanal may be present in all environmental compartments due to release or partitioning processes in the environment.

The substance is a neutral organic chemical that is slightly soluble in water and moderately volatile. The Henry's law constant (39.3 Pa·m^3/mol) indicates that it will be moderately volatile from water and moist soil. The substance is lipophilic with a log K_{OW} value of > 6.5. A carbon soil adsorption coefficient (K_{OC}) of 4,073.8 L/kg (REACH n.d.-b) indicates that the chemical will have slight mobility in soil and will preferentially adsorb to phases in the environment with high organic carbon content (including sediment and soil).

Based on physical and chemical properties, STP modelling (Struijs 1996), and fugacity modelling (US EPA 2017), Karanal is expected to mostly remain in air when released to the air compartment (> 80%). Following release to sewers, the chemical is expected to partly remain in water, partly volatilise, and partly partition to sediment and biosolids in STPs. Karanal may be emitted to the soil compartment through application of biosolids from STP processes. When applied to soils, it is expected to remain mostly in soil due to its low mobility.

Degradation

Karanal is expected to be persistent in the environment.

Based on slow hydrolysis rates and experimental ready and inherent biodegradation data on Karanal, its potential degradants and related chemicals, Karanal is persistent in water. While primary degradation or hydrolysis may slowly occur in environmental conditions, some of the expected transformation products formed through these processes are persistent. There are no measured half-life data for degradation of this chemical in sediment or soil. The chemical is not expected to be persistent in air based on its calculated half-life.

Abiotic degradation in water

Hydrolysis of Karanal is expected to be slow to negligible in environmentally relevant conditions. Based on a laboratory study according to OECD test guideline (TG) 111, a half-life of 30.8 days was estimated at pH 4 and 25°C, by extrapolation from data at 50–70°C (ECHA n.d.-a). However, the degree of hydrolysis was likely overestimated in this study. Quantification of hydrolysis products suggested that other dissipation processes such as volatilisation or binding to the test vessel were partly responsible for the disappearance of the test material. Results at pH 7 and 9 in buffered aqueous solution were inconclusive. However, a half-life of 10 days was measured in river water at pH 8.2 and 50°C, which is almost twice as long as the half-life at pH 4 and 50°C (ECHA n.d.-a). Based on this result, and the overestimation of hydrolysis seen at pH 4, the hydrolysis half-life of Karanal at pH 7–9 is expected to be > 60 days at environmentally relevant temperatures. No data on photodegradation in water were identified.

Ready biodegradability in water

Karanal was found to be not readily biodegradable in experimental studies. Degradation reached 12–34% after 28 days in an OECD TG 301 B (CO_2 evolution) study and up to 2% after 50 days in an OECD TG 301 F (O_2 consumption) study (ECHA n.d.-a; REACH n.d.-b; REACH n.d.-c). The test concentrations varied from 10-100 mg/L.

Inherent biodegradability in water

Available simulation test results for inherent biodegradability in water suggest that Karanal undergoes slow primary degradation. No evidence of significant ultimate biodegradation or mineralisation is available.

An inherent biodegradability test according to OECD TG 302 C (O_2 consumption) without pre-adaptation found 12% degradation after 28 days, and 18% degradation after 50 days (30 mg/L test concentration) (ECHA n.d.-a; REACH n.d.-b).

A degradation study in natural water (50 µg/L test concentration, 22°C) was conducted according to OECD TG 309 for 60 days. A thorough assessment of this study based on the confidential full study report highlighted deviations from the test guidelines (lack of controls, only one concentration tested) (ECHA n.d.-a). Disappearance of the test material was partly attributed to abiotic processes, likely adsorption to the test vessel and/or volatilisation. Based on these observations, a primary degradation half-life of 56 days at 22°C was estimated to be due only to biodegradation. As the test material was not radio-labelled and transformation products were not analysed, no further information on degradation pathways or ultimate degradation can be obtained from this study (ECHA n.d.-a).

Other compartments

No degradation data were identified for the sediment and soil compartments.
Karanal is expected to degrade quickly in the atmosphere through reaction with photogenerated hydroxyl radicals and ozone. Calculations performed assuming a typical hydroxyl radical concentration of 1.5×10^6 molecules/cm^3 resulted in a half-life of 1.04 h, while an ozone concentration of 7×10^{11} molecules/cm^3 resulted in a half-life of 38 min (US EPA 2017).

Potential degradation and metabolic pathways

Most degradation and metabolic models predict that the biotic transformation of Karanal likely starts with an oxidation step (-OH) on various positions of the dioxane or cyclohexene rings or their substituents. This is consistent with studies on the degradation of 1,4-dioxane, which starts with oxidation in the 2-position (Vainberg et al. 2006). Hydrolysis of the acetal to the corresponding aldehyde and diol is not predicted to be a biotic degradation pathway. However, other enzymatic transformations may lead to the formation of the 2,4-dimethyl-aldehyde 3-cyclohexene-1-carboxaldehyde (ECHA n.d.-a). Degradation studies mentioned under *Weight of evidence* below show that this aldehyde is persistent in water.

Analysis of transformation products of Karanal in degradation studies would allow a better understanding of potential primary degradation processes. However, the available data indicate that no significant mineralisation of the chemical is achieved in biodegradation tests.

Weight of evidence: persistence of related chemicals and potential degradation products of Karanal

Ready and inherent biodegradability tests on related chemicals indicate that both the cyclohexene and the substituted 1,3-dioxane moieties of Karanal are recalcitrant to biodegradation.

Two dioxanes identified by CAS numbers 80480-24-6 and 166301-21-9 (**Figure 2**) are substituted in the 2- and 5-positions, similar to Karanal. These substances are not readily biodegradable. Two degradation studies conducted with the first dioxane derivative (CAS number 80480-24-6) reached 17% degradation (OECD TG 301 B) and 7% degradation (ISO draft guideline, O_2 consumption) after 28 days (REACH n.d.-d). The degradation of the second dioxane derivative (CAS number 166301-21-9) reached 9% after 28 days (OECD TG 301 F). This substance was also found to be not inherently biodegradable in an OECD TG 302 C test (Modified MITI test (II)) (REACH n.d.-e).

Aldehydes **A** and **B** (**Figure 2**) contain a cyclohexene ring and are potential degradation products of Karanal and of its 4,6-isomer, respectively. Screening and simulation tests of mixtures of these substances with other isomers showed that they are not readily or inherently biodegradable. In an OECD TG 301 F test on a mixture of aldehyde **A** and its 3,5-dimethyl isomer **C** (**Figure 2**), degradation reached 0.75% after 28 d. In an OECD TG 309 test on a ^{14}C-labelled test material of the above mixture, no significant mineralisation to $^{14}CO_2$ was observed after 58 days. Primary degradation occurred and the degradation products were tentatively assigned to the corresponding carboxylic acids (REACH n.d.-f). Similarly, a mixture of aldehyde **B** and its 3,6-dimethyl isomer **D** (**Figure 2**) was found to be not readily biodegradable (0–4% degradation, 28 days, OECD TG 301 C and OECD TG 301 D tests) and not inherently biodegradable (mineralisation < 2% after 63 days in an OECD TG 309 test with a ^{14}C radio-labelled material) (REACH n.d.-g). All concentrations in the tests above, where reported, varied from 10–100 mg/L for ready biodegradation tests and 0.01–30 mg/L for inherent biodegradation tests.

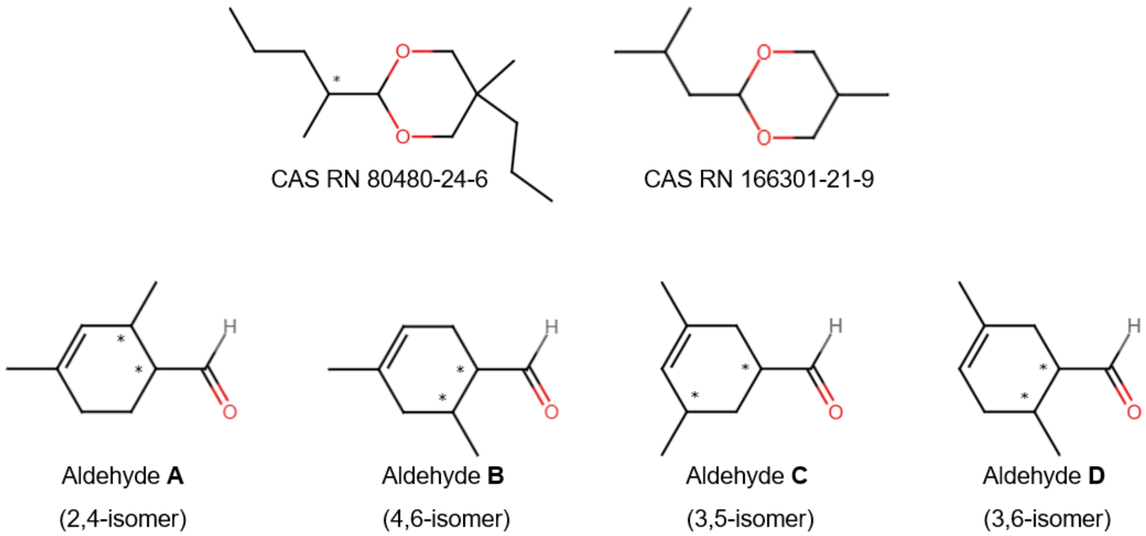


Figure 2. Structural formulae of Karanal related chemicals and potential degradation products tested in biodegradation studies: 5-methyl-2-(1-methylbutyl)-5-propyl-1,3-dioxane (CAS number 80480-24-6), 5-methyl-2-(2-methylpropyl)-1,3-dioxane (CAS number 166301-21-9), 2,4-dimethyl-3-cyclohexene-1-carboxaldehyde (aldehyde **A**), 4,6-dimethyl-3-cyclohexene-1-carboxaldehyde (aldehyde **B**), 3,5-dimethyl-3-cyclohexene-1-carboxaldehyde (aldehyde **C**), and 3,6-dimethyl-3-cyclohexene-1-carboxaldehyde (aldehyde **D**). Asterisks indicate chiral centres.

Bioaccumulation

Karanal is bioaccumulative in fish and earthworms. Experimental and calculated bioconcentration factors (BCFs) are above Australian categorisation thresholds for bioaccumulation in aquatic organisms (DCCEEW n.d.). A study in earthworms further supports the bioaccumulative characteristics of Karanal in soil dwelling organisms.

Experimental studies of the octanol-water partitioning coefficient using the HPLC method (OECD TG 117) indicate that the log K_{OW} for Karanal exceeds 6.5 (ECHA n.d.-a).

Measured kinetic BCFs for rainbow trout (*Oncorhynchus mykiss*) according to OECD TG 305 were found to be 2,171 L/kg wet weight (ww) and 9,406 L/kg ww, in flow through conditions at nominal concentrations of 0.003 mg/L and 0.03 mg/L, respectively. After correction for the growth rate of the fish and normalisation to a lipid content of 5%, these BCF values are adjusted to 1,892 and 9,893 L/kg ww, respectively. A steady state was reached within 47 days, and depuration over 35 days was more than 94% for both concentrations. The BCF value at the lower concentration is less reliable than at the higher concentration due to uncertainties in the measurements of the water concentrations (ECHA, n.d.-a).

Calculated BCF values for fish according to the Arnot-Gobas model were between 2,171 L/kg ww (with biotransformation) and 18,660 L/kg ww (no biotransformation), based on log K_{OW} values above 6.5 (US EPA 2017).

A 21 day bioaccumulation study with the earthworm *Eisenia fetida* following OECD TG 317 determined a kinetic biota-soil accumulation factor ($BSAF_k$) of 15.76 kg oc/kg lipid after normalisation to the organic and lipid content ("oc" refers to the organic content in soil and "lipid" refers to the lipid content in worms) (ECHA n.d.-a). A domestic bioaccumulation threshold is not available for BSAF endpoints. Lipid- and organic carbon-normalised BSAF values of 0.5 and above are considered an indication of high bioaccumulation potential for chemicals with log K_{OW} above 5.5 (ECHA 2023). Consequently, a $BSAF_k$ of 15.76 kg oc/kg lipid suggests that Karanal has the potential to strongly bioaccumulate in earthworms.

Environmental transport

No evidence of long range transport was found for Karanal.

No environmental monitoring studies were identified for the chemical. Monitoring data in remote regions of the world far from sources of release are not available.

Karanal is not expected to undergo long range transport in air. The chemical is moderately volatile but has a short predicted atmospheric half-life of about 1 hour (US EPA 2017). Karanal may adsorb to particulate matter, and the sorbed fraction may be resistant to atmospheric oxidation. However, the sorbed fraction is predicted to be less than 1% (US EPA 2017).

Although Karanal is persistent in water, evaporation of the substance is expected to limit its potential for long range transport in the aquatic environment, with calculated volatilisation half-lives from rivers and lakes of 4 h and 7.6 days, respectively (US EPA 2017).

Predicted environmental concentration (PEC)

Karanal has been identified in this evaluation as a PBT substance. It is not currently possible to derive a safe environmental exposure level for the chemical. Therefore, the environmental risks for this chemical cannot be characterised in terms of a risk quotient (RQ). As such a predicted environmental concentration (PEC) has not been calculated.

No domestic or international monitoring data are available for Karanal.

Environmental effects

Effects on aquatic life

Karanal is expected to cause toxic effects at low concentrations in aquatic organisms across multiple trophic levels.

Acute toxicity

The following measured median lethal concentration (LC50) and median effective concentration (EC50) values for freshwater model organisms across three trophic levels were retrieved from the REACH dossiers for Karanal (REACH n.d.-b; REACH n.d.-c) and from the SVHC report under EU REACH legislation (ECHA n.d.-a):

Taxon	Endpoint	Method
Fish	96 h LC50 ≤ 0.3 mg/L	*Cyprinus caprio* (common carp) semi-static conditions nominal concentrations OECD TG 203
Invertebrate	48 h EC50 (mobility) = 5.35 mg/L*	*Daphnia magna* (water flea) static conditions nominal concentrations OECD TG 202
Algae	72 h EC50 (growth) > 0.336 mg/L 72 h EC50 (yield) = 0.306 mg/L	*Raphidocelis subcapitata* (green algae) static conditions measured concentrations OECD TG 201

* Denotes an endpoint greater than the water solubility of the chemical

The reliability of the fish LC50 endpoint (0.3 mg/L) is limited due to the use of nominal concentrations and potential volatilisation of the test substance (ECHA n.d.-a). However, volatilisation would result in lower actual concentrations of Karanal in the test medium and; therefore, in a lower LC50 value. The LC50 endpoint of 0.3 mg/L based on nominal concentrations is considered sufficient evidence that the median lethal concentration is below the acute toxicity threshold of 1 mg/L.

Chronic toxicity

The following measured no observed effect concentration (NOEC) and 10% effective concentration (EC10) values for model organisms across three trophic levels were retrieved from the SVHC report under EU REACH legislation (ECHA n.d.-a):

Taxon	Endpoint	Method
Fish	32 d NOEC (mortality) = 0.03 mg/L	*Pimephales promelas* (fathead minnow) semi-static conditions measured concentrations (time-weighted average) OECD TG 210
Invertebrates	21 d NOEC (reproduction) = 0.096 mg/L	*Daphnia magna* (water flea) semi-static conditions measured concentrations OECD TG 211
Algae	72 h EC10 (growth) = 0.286 mg/L	*Raphidocelis subcapitata* (green algae) static conditions measured concentrations OECD TG 201

Effects on terrestrial life

A 14 d LC50 of 410.2 mg/kg soil (dry weight, dw) was determined for the earthworm *Eisenia fetida* (artificial soil, nominal concentrations, OECD TG 207) (REACH n.d.-b).

Effects on sediment dwelling life

There are no suitable data available to evaluate the effects of Karanal on sediment dwelling organisms.

Predicted no-effect concentration (PNEC)

Karanal has been identified as a bioaccumulative and environmentally persistent chemical. These hazard characteristics combined have the potential to result in a range of long term effects on organisms exposed to the chemical, which cannot be readily identified through standard toxicity testing. For such chemicals, it is not currently possible to estimate a safe exposure concentration. Therefore, a PNEC has not been derived for the substance.

Categorisation of environmental hazard

The categorisation of the environmental hazards of the assessed chemical according to Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals (EPHC 2009) is presented below.

Persistence

Persistent (P). Based on a lack of degradation or mineralisation in measured biotic and abiotic degradation studies in water, Karanal is categorised as Persistent.

Bioaccumulation

Bioaccumulative (B). Based on measured and calculated bioconcentration factors (BCF) in fish exceeding 2,000 L/kg and log K_{OW} values exceeding 4.2, Karanal is categorised as Bioaccumulative.

Toxicity

Toxic (T). Based on acute ecotoxicity values below 1 mg/L and chronic ecotoxicity values below 0.1 mg/L, Karanal is categorised as Toxic.

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:

- No domestic or international monitoring data are available for Karanal in surface water or air.
- Ecotoxicity data for the soil and sediment compartments are limited to a study in earthworms.

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