Fragrance chemicals used in very low volumes: Environment tier III assessment

08 March 2019

CAS Registry Numbers: 6379-73-3 and 52844-21-0

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 III because the Tier II assessment indicated that it needed further investigation. The report should be read in conjunction with the Tier II assessment.

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

Disclaimer

Acronyms & Abbreviations

Synopsis

The two chemicals in this assessment have known or potential industrial uses as fragrances. They were assessed in the Tier II environment assessment of fragrance chemicals with limited available environmental data and both were recommended for Tier III assessment under the IMAP framework (NICNAS, 2018a). A Tier III human health assessment of both chemicals has been published (NICNAS, 2018b).

The Tier II environmental risk characterisation indicated potentially unreasonable risks for both chemicals based on estimated environmental exposure concentrations that exceeded the no unacceptable adverse effect concentrations for aquatic life. In the absence of other information, the assessment relied on default assumptions regarding the annual introduction volume for industrial chemicals. The default introduction volume was used to estimate the environmental exposure that would result from use of these chemicals as fragrance ingredients in personal care and household cleaning products. It was noted that relying on default introduction volumes could result in an overestimation of risks to aquatic life. A key finding of the Tier II assessment was that further refinement of the risk characterisation for both chemicals is dependent on the availability of new information which includes the volumes of each chemical that are used as fragrance ingredients.

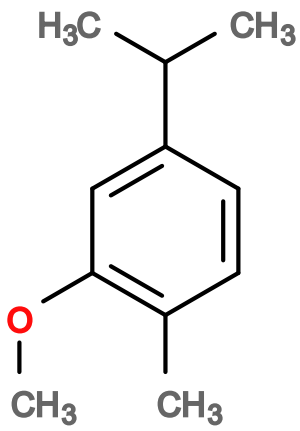
Rationale for Tier III Assessment

Following consultation with industry, NICNAS received new information on the volumes of these chemicals that are used globally as fragrance ingredients. This new information shows that the environmental emissions of both chemicals that result from their use as fragrance ingredients were overestimated in the Tier II environment assessment. The conclusions regarding potential risks to the environment from industrial uses of these two chemicals can be modified based on this new information and updating the risk characterisation for both chemicals is the focus of this Tier III assessment.

Chemical Identity

Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)- is more commonly known as carvacryl methyl ether or carvacrol methyl ether. It is a terpenoid natural product which is present as a minor constituent of the essential oils extracted from the perennial herbs, oregano and thyme (G De Mastro, et al., 2017; Wesołowska, et al., 2016).

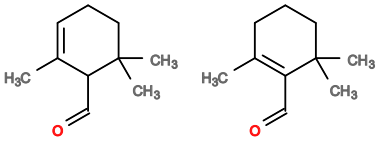
CAS RN	6379-73-3
Chemical Name	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-
Synonyms	carvacryl methyl ether

	carvacrol methyl ether 5-isopropyl-2-methylanisole
Structural Formula	
Molecular Formula	$C_{11}H_{16}O$
Molecular Weight (g/mol)	164.24
SMILES	c1(C)c(OC)cc(C(C)C)cc1

The chemical assigned CAS RN 52844-21-0 is an incompletely defined substance according to the Chemical Abstracts Service. There are four possible constitutional isomers of this substance based on differences in the position of the alkene unit in the cyclohexene ring. However, the substance is generally taken to be an unspecified mixture of only two of these isomers, alpha-cyclocitral (CAS RN 432-24-6) and beta-cyclocitral (CAS RN 432-25-7) (US EPA, 1979). Various mixtures of alpha- and beta-cyclocitral have been prepared using different synthetic methods described in the research and patent literature (Gedye, et al., 1971; Janitschke and Hoffman, 1982). Alpha- and beta-cyclocitral are volatile terpenoids which are aroma chemicals present in a range of fruits, vegetables and plants (Condurso, et al., 2016).

The chemical structure information provided for this substance in the Tier II environment assessment has been updated here to indicate that it is considered to be a mixture of alpha- and beta-cyclocitral:

CAS RN	52844-21-0
Chemical Name	Cyclohexenecarboxaldehyde, 2,6,6-trimethyl-
Synonyms	alpha(beta)-cyclocitral cyclocitral

	2,6,6-trimethylcyclohexenecarboxaldehyde
Structural Formula	
Molecular Formula	$C_{10}H_{16}O$
Molecular Weight (g/mol)	152.23
SMILES	C1(C)(C)C(C=O)C(C)=CCC1 C1(C)(C)C(C=O)=C(C)CCC1

Import, Manufacture and Use

Carvacryl methyl ether is used in very low volumes worldwide as a fragrance chemical. There are no known current industrial uses of alpha(beta)-cyclocitral.

According to information provided by the International Fragrance Association (IFRA), less than 10 kilograms per annum of carvacryl methyl ether was used globally as a fragrance ingredient in the most recent reporting period (NICNAS, 2018b).

There are no reported uses of alpha(beta)-cyclocitral as a fragrance ingredient in databases of cosmetics and there was no reported use of this chemical in the most recent global survey of members of IFRA. Beta-cyclocitral (CAS RN 432-25-7) is used as a fragrance chemical, but only in very low volumes (up to 1 kilogram per annum globally) (NICNAS, 2018b).

No other industrial uses for carvacryl methyl ether or alpha(beta)-cyclocitral have been identified.

Risk Characterization

Use of carvacryl methyl ether and alpha(beta)-cyclocitral as fragrance ingredients does not pose an unreasonable risk to the environment.

Information provided to NICNAS on the global volume of use of certain fragrance ingredients shows that carvacryl methyl ether and alpha(beta)-cyclocitral are either used in very low volumes or they no longer have significant uses as fragrance ingredients. Based on this new information, emissions of carvacryl methyl ether to the environment from its use as a fragrance ingredient are negligible. There are no reported current uses of alpha(beta)-cyclocitral and only very low volume uses of one of its constituent isomers. The release of alpha- and beta-cyclocitral into the environment will, therefore, be dominated by emissions from their non-industrial uses (e.g. use as flavouring agents) and from natural sources.

Based on the available information, emissions of the chemicals in this group to the environment from their use as fragrance ingredients are negligible. There is, therefore, no longer a concern that known industrial uses of these chemicals will result in their emission to surface waters at levels that are harmful to aquatic life. As these chemicals do not have the characteristics of PBT substances there are no remaining concerns for the environment regarding their use as fragrance ingredients in Australia.

Recommendations

No further assessment of the chemicals in this group is required unless additional industrial uses resulting in substantial emissions to the environment are identified.

References

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Last update 8 March 2019

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