Simple esters of geraniol and nerol: Human health tier II assessment

30 June 2017

Chemicals in this assessment

Chemical Name in the Inventory	CAS Number
2,6-Octadien-1-ol, 3,7-dimethyl-, benzoate, (E)-	94-48-4
Benzeneacetic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-	102-22-7
2,6-Octadien-1-ol, 3,7-dimethyl-, formate, (E)-	105-86-2
2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)-	105-87-3
2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (E)-	105-90-8
2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (Z)-	105-91-9
Butanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-	106-29-6
Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-	109-20-6
2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-	141-12-8

Chemical Name in the Inventory	CAS Number
Butanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-	999-40-6
2,6-Octadien-1-ol, 3,7-dimethyl-, formate, (Z)-	2142-94-1
Propanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (Z)-	2345-24-6
Propanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-	2345-26-8
Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (Z)-	3915-83-1
Butanoic acid, 3-oxo-, 3,7-dimethyl-2,6-octadienyl ester, (E)-	10032-00-5
Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-	10032-02-7
Pentanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-	10402-47-8
Pentanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-	10522-33-5
2,6-Octadien-1-ol, 3,7-dimethyl-, acetate	16409-44-2
2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate	27751-90-2
Octanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-	51532-26-4
2,6-Octadien-1-ol, 3,7-dimethyl-, formate	61759-63-5
Nonanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-	68039-29-2
Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-	68310-59-8

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

ACRONYMS & ABBREVIATIONS

Grouping Rationale

This group is composed of various esters of geraniol and its isomeric forms: nerol and citrol (a mix of geraniol and nerol). These isomers are toxicologically similar (See Geraniol and related compounds; NICNAS). The chemicals are known to be used in perfumes (see **Use** section). In addition, upon exposure, it is expected that the chemicals will be hydrolysed into geraniol and the corresponding carboxylate. The carboxylates associated with the esters in this group are of low toxicity. On the basis of similar uses and that the toxic effects of the chemicals are dependent on the formation of geraniol or nerol, the assessment of these chemicals as a group is considered appropriate.

Import, Manufacture and Use

Australian

Geranyl acetate, geranyl formate and geranyl propanoate were reported to have use as flavouring agents in tobacco at concentrations of ≤0.0001 % of the product weight (Phillip Morris Ltd, 2014).

The chemicals geranyl acetate, geraniol formate and nerol acetate (CAS numbers 105-87-3, 105-86-2, and 141-12-8, respectively) have reported uses in cleaning agents and coatings in marine applications.

International

The following international uses have been identified through: the European Union (EU) Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) dossiers; Galleria Chemica; the European Commission Cosmetic Ingredients and Substances (CosIng) database; the International Fragrance Association (IFRA); the United States (US) Personal Care Products Council International Nomenclature of Cosmetic Ingredients (INCI) Dictionary; the US National Library of Medicine's Hazardous Substances Data Bank (HSDB); Joint FAO/WHO Expert Committee on Food Additives (JECFA); the Good Scents Company and Monographs on Fragrance Raw Materials.

The chemicals have reported cosmetic use as fragrance ingredients.

The chemicals have reported non-industrial use as flavouring agents.

Restrictions

Australian

No known restrictions have been identified for any chemicals in this assessment.

International

Geranyl acetate is listed by the United States Food and Drug Administration (US FDA) as a synthetic flavouring substance that is generally recognised as safe (GRAS) for its intended use (21 CFR 582.60).

Geranyl acetate was assigned with an acceptable dietary intake (ADI) value of 0–0.5 mg/kg (Opdyke, 1979).

Existing Worker Health and Safety Controls

Hazard Classification

The chemicals are not listed on the Hazardous Chemical Information System (HCIS) (Safe Work Australia).

Exposure Standards

Australian

No specific exposure standards are available.

International

No specific exposure standards are available.

Health Hazard Information

Limited information is available for some of the chemicals in this group. In the absence of hazard data, the information for geraniol, nerol, and citrol (CAS numbers 106-24-1, 106-25-2, and 624-15-7, respectively) and the corresponding aliphatic carboxylic acids will be considered relevant, given the expected metabolic profile of the chemicals (see **Toxicokinetics** section) (NICNAS).

While the carboxylic acid constituents of the esters generally have local irritant effects, these are not relevant to the esters which are hydrolysed following absorption to carboxylate ions under physiological pH conditions.

Toxicokinetics

The chemicals in this group are expected to hydrolyse to geraniol and the anion of the corresponding aliphatic carboxylic acid (specifically butyric acid, hexanoic acid, acetoacetic acid, phenylacetic acid, perlargonoic acid, octanoic acid, pentanoic acid, butanoic acid, benzoic acid, formic acid, propanoic acid and acetic acid) (WHO, 1998).

The metabolic profile and hazards for geraniol has been discussed in a previous NICNAS Tier II assessment (NICNAS). Geraniol and its isomers were assessed as irritants (skin and eyes) and skin sensitisers (NICNAS).

The assessment for benzoic acid and some of the corresponding aliphatic carboxylic acids indicates that these metabolites are not likely to cause systemic toxicological concerns as the main critical health effects of these chemicals are local effects due to their pH levels (NICNASa; NICNASb; NICNASc; NICNASd).

Acetoacetic acid (CAS No. 541-50-4) is a weak acid produced by the liver, but under conditions of poor metabolism, may cause systemic toxicity by excessive fatty acid breakdown (PubChem).

Phenylacetic acid (CAS No. 103-82-2) is a nitrogen binding agent (PubChem) that is rapidly absorbed by the buccal tissues/membranes. It is vastly distributed throughout the human body and excreted as a glutamine conjugate; therefore, it has no bio-accumulation potential—systemic toxicity at low levels was not seen (REACHb).

Overall, considering the levels of use and type of exposures, the metabolites are not considered systemically hazardous.

Acute Toxicity

Oral

Available information shows that the chemicals in this group have low oral acute toxicity.

In a study conducted in Fischer 344 (F344/N) rats and B6C3F1 mice (n = 5/sex/dose), geranyl acetate (in corn oil) was administered at a single dose of either 500, 1000, 2000, 4000 or 8000 mg/kg bw. No controls were used in this study. All the rats in the high dose group died two days post-administration. No mortality occurred in the other dose groups. All dosed rats were inactive immediately after dosing. All the female mice and most of the male mice (4/5 animals) in the high dose group died by the third day post-administration. All mice from the1000 mg/kg bw group to the high dose group were inactive after dosing (NTP, 1987). The median lethal dose (LD50) value in rats was greater than 4000 mg/kw bw.

In a study conducted according to OECD TG 401, Osborne-Mendel rats (n =5/sex/dose) were administered geranyl butyrate (vehicle not specified) by gavage (doses were not provided) and observed for 14 days. Observed sub-lethal effects included depressed behaviour and coma at the highest dose group. All treated rats died after 4 days of dose administration. An oral LD50 of 10,660 mg/kg bw was reported (REACHa).

The oral LD50 values for the following chemicals were reported (Opdyke, 1979; WHO, 1998; EFSA, 2005; Tisserand & Young, 2014):

- geranyl acetate: 6330 mg/kg;

- geranyl acetoacetate: >5000 mg/kg;
- geranyl phenylacetate: >5000 mg/kg;
- geranyl benzoate: >5000 mg/kg;
- geranyl propionate: >5000 mg/kg;
- geranyl formate: >6000 mg/kg;
- geranyl isovalerate: >5000 mg/kg;
- geranyl hexanoate: >5000 mg/kg;
- geranyl isobutyrate: >5000 mg/kg; and
- neryl isovalerate: >5000 mg/kg.

Dermal

Available information shows that the chemicals in this group have low dermal acute toxicity.

The dermal LD50 values for the following chemicals were reported (Opdyke, 1979; WHO, 1998; Tisserand & Young, 2014; REACHa):

- geranyl benzoate: >5000 mg/kg;
- geranyl phenylacetate: >5000 mg/kg;
- geranyl propionate: >5000 mg/kg;
- geranyl formate: >5000 mg/kg;
- geranyl isovalerate: >5000 mg/kg;
- neryl formate: 5000 mg/kg;
- neryl isovalerate: >5000 mg/kg; and
- geranyl butyrate: 5000 mg/kg.

Inhalation

No data are available for the chemicals.

Corrosion / Irritation

Skin Irritation

Based on the available animal and human data, the chemicals in this group are not considered to be skin irritants.

Geranyl isobutyrate (100 %) and neryl isovalerate (100 %) were mildly irritating to intact or abraded rabbit skin when applied under occlusion for 24 hours (Opdyke, 1979).

Reports on the following chemicals indicate that these did not cause irritation when applied to rabbit skin (Opdyke, 1979; Tisserand & Young, 2014; REACHa):

- geranyl benzoate;
- geranyl propanoate (undiluted);
- geranyl phenylacetate;
- geranyl isovalerate;
- geranyl formate; and
- geranyl butyrate.

Eye Irritation

Based on the available animal data from geranyl formate, the chemicals in this group are considered to be no more than slight eye irritants. Slight irritation was observed when geranyl formate was instilled into the eyes of rabbits for 72 hours. Irritation was fully reversible after 72 hours (REACHa).

Observation in humans

Geranyl formate (2 %) produced mild skin irritation when tested on 25 volunteers (Tisserand & Young, 2014).

Reports on the following chemicals indicate that these did not cause irritation in a 48-hour human patch test (Opdyke, 1974; REACHa):

- geranyl benzoate (2 % in petrolatum);
- geranyl isovalerate (2 % in petrolatum);
- geranyl phenylacetate (4% in petrolatum);
- geranyl isobutyrate (10 % in petrolatum);
- geranyl butyrate (4 % in petrolatum); and
- neryl isovalerate (6 % in petrolatum).

Geranyl propionate (4 %) was also reported as not causing skin irritation when tested on 25 volunteers (Tisserand & Young, 2014).

Sensitisation

Skin Sensitisation

The available data are considered insufficient for a definite conclusion on the sensitising potential of the chemicals in this group. Geraniol and its isomers are known to be skin sensitisers (NICNAS).

In a modified Draize study, geranyl formate did not cause sensitising effects on guinea pig skin at a concentration of 20 % during the challenge phase. The induction concentration was not provided (Tisserand & Young, 2014).

Observation in humans

Geranyl acetate (4 % in petrolatum) was not considered sensitising based on a maximisation test conducted on 25 volunteers. However, hypersensitivity was observed in certain individuals.

Negative results were observed for the following chemicals (Opdyke, 1974; REACHa):

- geranyl benzoate (2 % in petrolatum);
- geranyl propanoate (4 %);
- geranyl formate (2 %);
- geranyl isovalerate;
- geranyl isobutyrate (10% in petrolatum);and
- geranyl butyrate (4% in petrolatum).

Repeated Dose Toxicity

Oral

Based on the available data, the chemicals in this group are not expected to cause systemic effects following repeated oral exposure.

In a 14-day study conducted in F344/N rats and B6C3F1 mice (n = 5/sex/dose), geranyl acetate was administered by gavage at doses of 0, 62, 125, 250, 500 or 1000 mg/kg bw/day in rats; and 0, 125, 250, 500, 1000 or 2000 mg/kg bw/day in mice. In rats, no mortality or any treatment-related effects occurred in any dose groups. In mice, three females in the 2000 mg/kg bw/day group died. In the 2000 mg/kg bw/day mice group, one male showed thickened duodenal wall while three females showed 'thickened wall of the cardia stomach'. Mice dosed at 1000 mg/kg bw/day were inactive but returned to normal 24 hours post-administration. These effects were determined to be treatment-related (NTP, 1987). A no observed adverse effect level (NOAEL) value was not reported in this study.

In a 17-week study, geranyl acetate, at concentrations of up to 10000 ppm in their diet did not cause any toxic effects in rats (Opdyke, 1974).

In a two-year study (5 days/week) conducted in F344/N rats and B6C3F1 mice (n = 50/sex/dose), geranyl acetate (in corn oil) was administered by gavage at doses of either 0, 1000 or 2000 mg/kg bw/d in rats; and 0, 500 or 1000 mg/kg bw/d in mice. High mortality rates were observed in rats (high dose males) and mice (high dose males and all treated females). However, the high mortality rate in the high dose mouse group was considered due to an accidental administration of 2800 mg/kg bw of the chemical for three days during week 91 of the study. The mean body weights of the high dose rats and mice were lower compared to controls throughout most of the study. In mice, treatment-related increase of cytoplasmic vacuolisation in the liver and kidneys were observed (NTP, 1987). A no observed adverse effect level (NOAEL) value was not reported from this study.

Dermal

No data are available.

Inhalation

No data are available.

Genotoxicity

Based on the negative results of the available in vitro and in vivo data (WHO, 1998), geranyl acetate is not considered to be genotoxic. Geraniol and its isomers are also not considered to be genotoxic (NICNAS).

Negative results were found in in vitro tests including (WHO, 1998):

- Ames test in *Salmonella typhimurium* strains TA1535, TA1537, TA1538, TA98, TA100; with and without metabolic activation;
- rec-assay in *Bacillus subtilis*;
- hypoxanthine phosphoribosyl transferase (HGPRT) gene mutation assay and chromosomal aberration assay in Chinese hamster ovary (CHO) cells; and
- unscheduled DNA synthesis in rat primary hepatocytes.

Negative results were found in in vivo tests including (WHO, 1998):

- micronucleus and chromosomal aberration assays in mouse bone marrow;
- unscheduled DNA synthesis in male F344 rats; and
- sex-linked recessive lethal assay in *Drosophila melanogaster*;

Geranyl phenylacetate has been evaluated as having 'no safety concern for genotoxicity' by European Food Safety Authority (EFSA, 2009).

Carcinogenicity

The available two-year study showed that geranyl acetate is not likely to be carcinogenic. Based on the available genotoxicity data, geraniol and its isomers are also not considered likely to be carcinogenic.

In a two-year study (five days per week) conducted in F344/N rats (n = 50/sex/dose), geranyl acetate (in corn oil) was administered by gavage at doses of either 0, 1000 or 2000 mg/kg bw/day. Squamous cell papillomas and carcinomas on the skin were observed in rats dosed at 1000 mg/kg bw/day. However, the overall incidence of all epidermal tumours was not different among all groups (NTP, 1987).

Geranyl phenylacetate has been evaluated as having 'no safety concern for carcinogenicity' by EFSA (EFSA, 2009).

Reproductive and Developmental Toxicity

No data are available for the chemicals in this group. Given that geraniol and its isomers are not considered to be specific reproductive or developmental toxins (NICNAS), the potential of the chemicals in this group to cause reproductive and developmental effects are considered to be unlikely.

Risk Characterisation

Critical Health Effects

Based on the available hazard information, the chemicals in this group do not have any critical health effects for risk characterisation.

Public Risk Characterisation

Although the public could be exposed to the chemicals through potential cosmetic uses, the chemicals are not considered to pose an unreasonable risk to public health on the basis of their low hazard profile.

Occupational Risk Characterisation

During product formulation, dermal, ocular and inhalational exposure may occur, particularly where manual or open processes are used. These could include transfer and blending activities, quality control analysis, and cleaning and maintaining equipment. Worker exposure to the chemicals at lower concentrations could also occur while using formulated products containing the chemicals. The level and route of exposure will vary depending on the method of application and work practices employed.

The chemicals in this group have low hazard; therefore, the chemicals are not considered to pose an unreasonable risk to workers.

NICNAS Recommendation

Current chemical regulatory measures are considered adequate to protect public and workers' health and safety, provided that all requirements are met under workplace health and safety, and poisons legislation as adopted by the relevant state or territory. No further assessment is required.

Regulatory Control

Public Health

Products containing the chemicals should be labelled in accordance with state and territory legislation.

Work Health and Safety

Given the critical health effects, the risks to workers from these chemicals are not considered to be unreasonable. The chemicals in this group currently have no hazard classification for worker health and safety; this is considered appropriate based on the available data.

Advice for consumers

Products containing the chemicals should be used according to the instructions on the label.

Advice for industry

Control measures

Control measures to minimise any risks from oral, inhalation, dermal and occular exposure to the chemicals should be implemented in accordance with the hierarchy of controls. Approaches to minimise risk include substitution, isolation and engineering controls. Measures required to eliminate, or minimise risk arising from storing, handling and using a hazardous chemical depend on the physical form and the manner in which the chemicals are used. Examples of control measures that could minimise the risk include, but are not limited to:

- minimising manual processes and work tasks through automating processes;
- work procedures that minimise splashes and spills;
- regularly cleaning equipment and work areas; and

- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with the chemicals.

Guidance on managing risks from hazardous chemicals are provided in the *Managing risks of hazardous chemicals in the workplace—Code of practice* available on the Safe Work Australia website.

Personal protective equipment should not solely be relied upon to control risk and should only be used when all other reasonably practicable control measures do not eliminate or sufficiently minimise risk. Guidance in selecting personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

Obligations under workplace health and safety legislation

Information in this report should be taken into account to help meet obligations under workplace health and safety legislation as adopted by the relevant state or territory. This includes, but is not limited to:

- ensuring that hazardous chemicals are correctly classified and labelled;
- ensuring that (material) safety data sheets ((M)SDS) containing accurate information about the hazards (relating to both health hazards and physicochemical (physical) hazards) of the chemicals are prepared; and
- managing risks arising from storing, handling and using a hazardous chemical.

Your work health and safety regulator should be contacted for information on the work health and safety laws in your jurisdiction.

Information on how to prepare an (M)SDS and how to label containers of hazardous chemicals are provided in relevant codes of practice such as the *Preparation of safety data sheets for hazardous chemicals—Code of practice* and *Labelling of workplace hazardous chemicals—Code of practice*, respectively. These codes of practice are available from the Safe Work Australia website.

A review of the physical hazards of these chemicals has not been undertaken as part of this assessment.

References

European Commission Cosmetic Ingredients and Substances (CosIng) database. Accessed January 2017 at **http://ec.europa.eu/growth/tools-databases/cosing/**

European Food Safety Authority (EFSA) Journal 2005. Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Materials in contact with Food (AFC) on a request from the Commission related to Flavouring Group Evaluation 10: Accessed August 2017 at

European Food Safety Authority (EFSA) Journal 2009. Scientific Opinion of the Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids (CEF). Flavouring Group Evaluation 53 Revision 1. Accessed August 2017 at **http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2009.1024/epdf**

Galleria Chemica. Accessed February 2017 at **http://jr.chemwatch.net/galleria/**

Globally Harmonised System of Classification and Labelling of Chemicals (GHS) United Nations, 2009. Third edition. Accessed at **http://www.unece.org/trans/danger/publi/ghs/ghs_rev03/03files_e.html**

Hazardous Substances Data Bank (HSDB). National Library of Medicine. Accessed February 2017 at **http://toxnet.nlm.nih.gov**

International Fragrance Association (IFRA) Survey: Transparency List 2011. Accessed February 2017 at **http://www.ifraorg.org/en/ingredients**.

National Center for Biotechnology Information. PubChem Compound Database. Accessed August 2017 at **https://pubchem.ncbi.nlm.nih.gov/**

National Industrial Chemical Notification and Assessment Scheme (NICNAS). Human health Tier II assessment for geraniol and related compounds. Australian Government Department of Health. Accessed March 2017 at **https://www.nicnas.gov.au**

National Industrial Chemical Notification and Assessment Scheme (NICNASa). Human health Tier II assessment for benzoic acid (CAS No. 65-85-0). Australian Government Department of Health. Accessed February 2017 at **http://www.nicnas.gov.au**

National Industrial Chemical Notification and Assessment Scheme (NICNASb). Human health assessment for formic acid. CAS registry number: 64-18-6. Australian Government Department of Health and Ageing. Accessed February 2017 at **www.nicnas.gov.au**

National Industrial Chemical Notification and Assessment Scheme (NICNASc). Human Health Tier II Assessment for propanoic acid (CAS No. 79-09-4). Australian Government Department of Health. Accessed May 2015 at **http://www.nicnas.gov.au**

National Industrial Chemicals Notification and Assessment Scheme (NICNASd). Inventory Multi-Tiered and Prioritisation (IMAP): Human Health Tier II Assessment for acetic acid (Cas No. 64-19-7). Available at **http://www.nicnas.gov.au**

National Toxicology Program (NTP) 1987. NTP Technical Report on the Carcinogenesis Studies of Food Grade Geranyl Acetate (71% Geranyl Acetate, 29% Citronellyl Acetate) (CAS No 105-87-3). Accessed February 2017 at **https://ntp.niehs.nih.gov/ntp/htdocs/lt_rpts/tr252.pdf**

Opdyke DL 1979. Monographs on fragrance raw materials. Food Cosmet Toxicol. 1979 Aug;17(4):357-90.

Personal Care Product Council International Nomenclature of Cosmetic Ingredients (INCI) Dictionary. Accessed February 2017 at **http://www.ctfa-gov.org/jsp/gov/GovHomePage.jsp**

Phillip Morris Ltd. Australia Ingredients Report: Composite List of Tobacco Ingredients for reporting period (March 1, 2013 to March 1, 2014) (pursuant to Clause 6.3(ii) of the Agreement between the Commonwealth and the Manufacturers dated December 20, 2000). Accessed on February 2017 at **http://www.health.gov.au/internet/main/publishing.nsf/Content/health-tobacco-ingredients-philip-2014**

Registration, Evaluation, Authorisation and Restriction of Chemicals (REACHa) Dossier for geranyl acetate (CAS No 105-87-3). Accessed February 2017 at **http://echa.europa.eu/information-on-chemicals/registered-substances**.

Registration, Evaluation, Authorisation and Restriction of Chemicals (REACHb) Dossier for phenylacetic acid (CAS No. 103-82-2). Accessed August 2017 https://echa.europa.eu/substance-information/-/substanceinfo/100.002.862

Safe Work Australia. Hazardous Chemicals Information System (HCIS). Accessed February 2017 at **http://hcis.safeworkaustralia.gov.au/HazardousChemical**

The Good Scent Company data on Geraniol compounds (CAS No.: various). Accessed August 2017 at **www.thegoodscentscompany.com/**

Tisserand R, Young R 2014. Essential Oil Safety: A Guide for Health Care Professionals. 2nd edn. Churchill Livingstone, St. Louis,

US Food& Drug Administration (US FDA) 21CFR582.60. Code of Federal Regulations, Title 21, Volume 6. Revised April 1, 2016. Part 582 - Substances Generally Recognized as Safe (GRAS). Accessed February 2017 at **http://www.accessdata.fda.gov/scripts/cdrh/cfdocs/cfcfr/cfrsearch.cfm?fr=582.60**

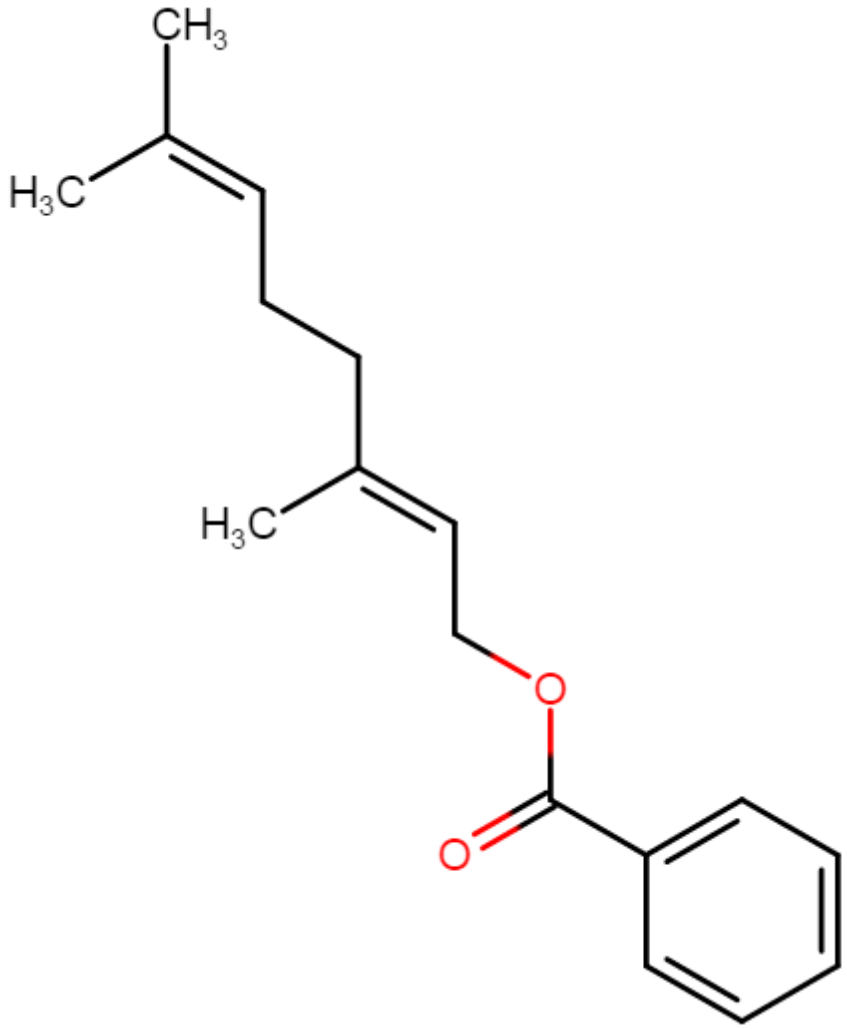
World Health Organisation (WHO) International Programme on Chemical Safety 1998. Safety Evaluation of Certain Food Additives and Contaminants. WHO Food Additives Series 40. Accessed on february 2017 at **http://www.inchem.org/documents/jecfa/jecmono/v040je15.htm**

World Health Organization (WHO) Joint FAO/WHO Expert Committee on Food Additives (JECFA) 1999. Evaluation of certain food additives and contaminants: forty-ninth report of the Joint FAO/WHO Expert Committee on Food Additives (WHO Technical Report Series 884). Available at **http://apps.who.int/iris/bitstream/10665/42142/1/WHO_TRS_884.pdf**

Last Update 30 June 2017

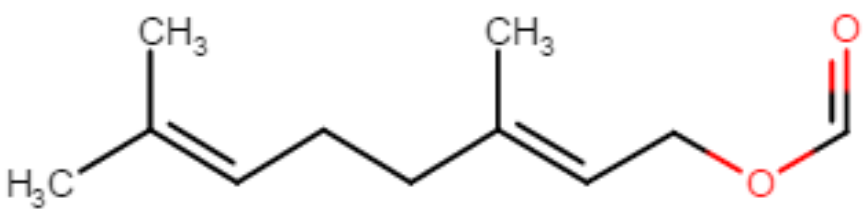
Chemical Identities

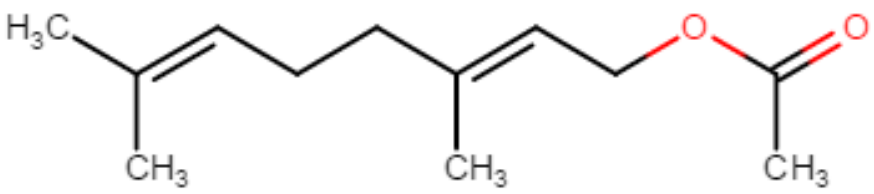
Chemical Name in the	**2,6-Octadien-1-ol, 3,7-dimethyl-, benzoate, (E)-**

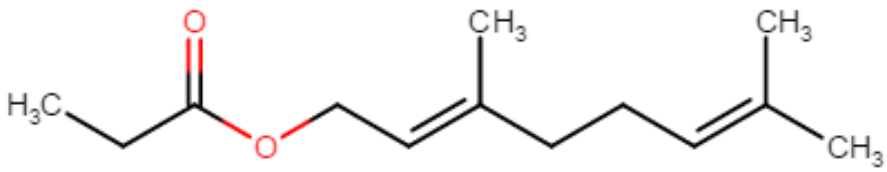
Inventory and Synonyms	geranyl benzoate
CAS Number	94-48-4
Structural Formula	
Molecular Formula	C17H22O2
Molecular Weight	258.36

Chemical Name in the Inventory and Synonyms	**Benzeneacetic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-** 3,7-Dimethyl-2,6-octadien-1-yl phenylacetate, (E)- Acetic acid, phenyl-, 3,7-dimethyl-2,6-octadienyl ter,(E)- Geranyl phenyl acetate
CAS Number	102-22-7
Structural Formula	

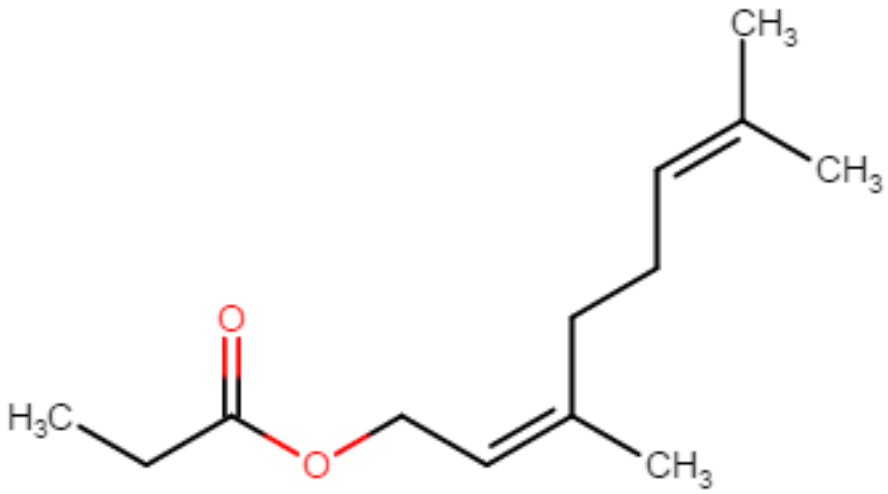
	
Molecular Formula	C18H24O2
Molecular Weight	272.38

Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, formate, (E)-** 3,7-dimethyl-2,6-octadienyl methanoate, (E)- geranyl formate
CAS Number	105-86-2
Structural Formula	
Molecular Formula	C11H18O2
Molecular Weight	182.26

Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)-** 3,7-dimethyl-2,6-octadienyl acetate, (E)- geranyl acetate
CAS Number	105-87-3
Structural Formula	
Molecular Formula	C12H20O2
Molecular Weight	196.29

Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (E)-** geranyl propionate
CAS Number	105-90-8
Structural Formula	
Molecular Formula	C13H22O2
Molecular Weight	210.31

Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (Z)-** neryl propionate
CAS Number	105-91-9

Structural Formula	
Molecular Formula	C13H22O2
Molecular Weight	210.31

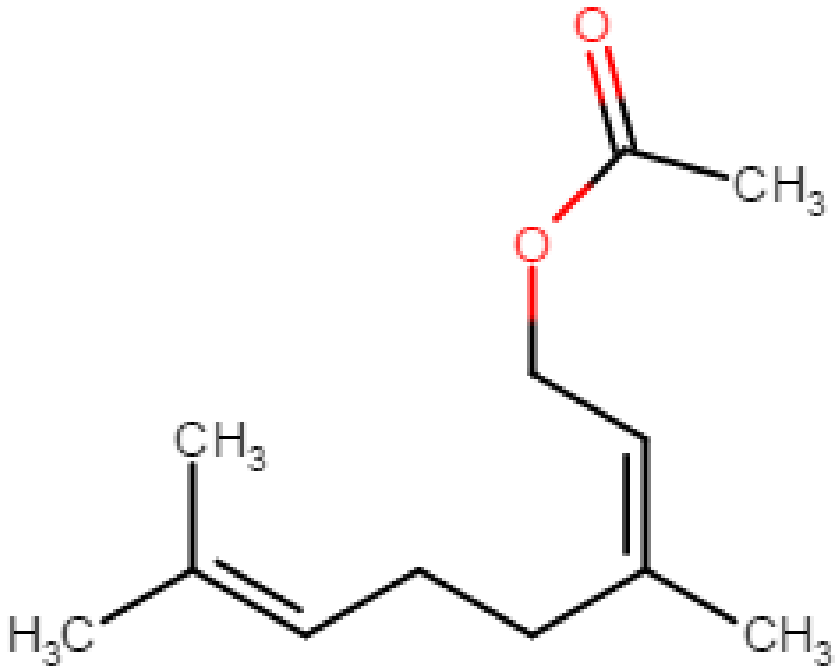
Chemical Name in the Inventory and Synonyms	**Butanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-** 3,7-Dimethyl-2,6-octadienyl butyrate, (E)- Geranyl butyrate
CAS Number	106-29-6
Structural Formula	

	
Molecular Formula	C14H24O2
Molecular Weight	224.34

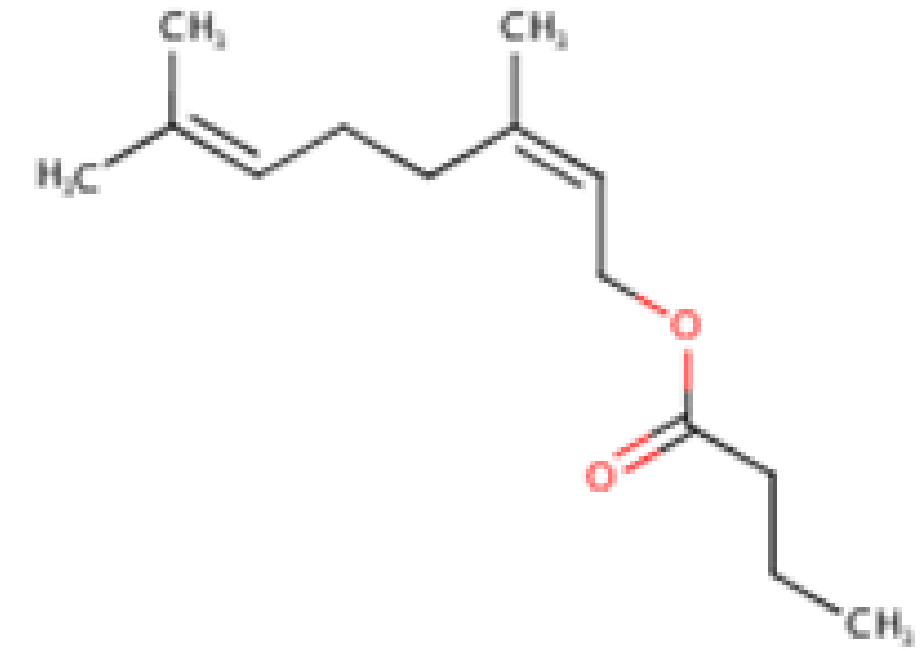
Chemical Name in the Inventory and Synonyms	**Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-** Geranyl isovalerate
CAS Number	109-20-6
Structural Formula	

	
Molecular Formula	C15H26O2
Molecular Weight	238.37

Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-** neryl acetate
CAS Number	141-12-8
Structural Formula	

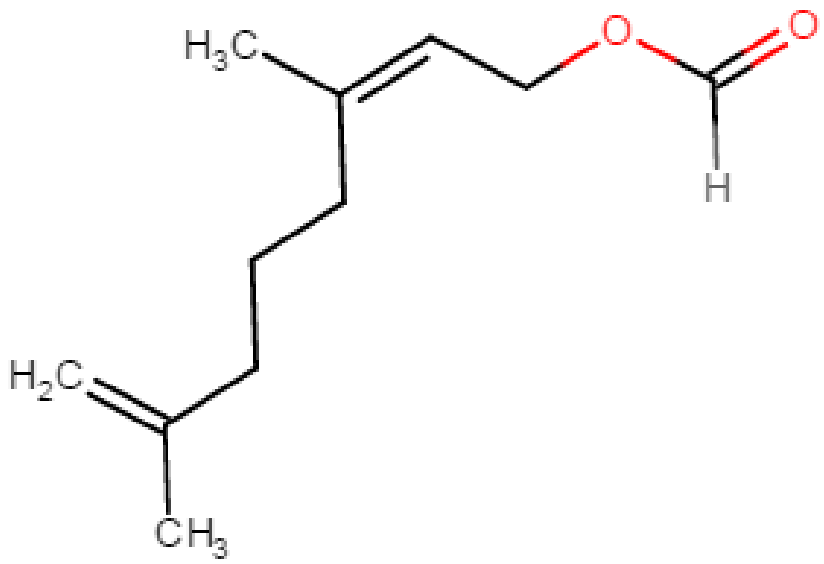
	
Molecular Formula	C12H20O2
Molecular Weight	192.29

Chemical Name in the Inventory and Synonyms	**Butanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-** Neryl butyrate
CAS Number	999-40-6
Structural Formula	

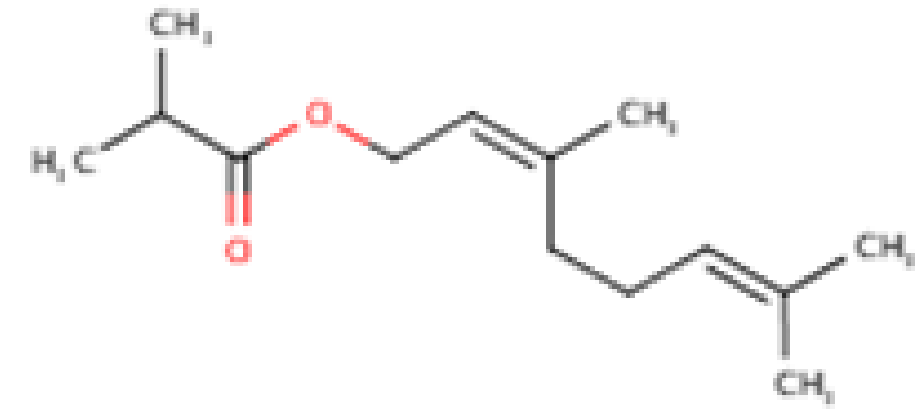


Molecular Formula	C14H24O2
Molecular Weight	224.34

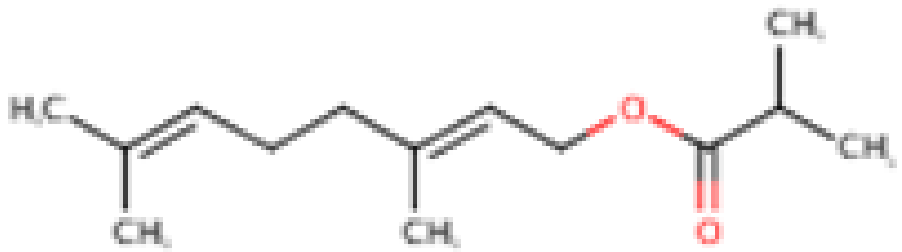
Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, formate, (Z)-** neryl formate
CAS Number	2142-94-1
Structural Formula	

	
Molecular Formula	C11H18O2
Molecular Weight	182.26

Chemical Name in the Inventory and Synonyms	**Propanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (Z)-** Isobutyric acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-
CAS Number	2345-24-6
Structural Formula	

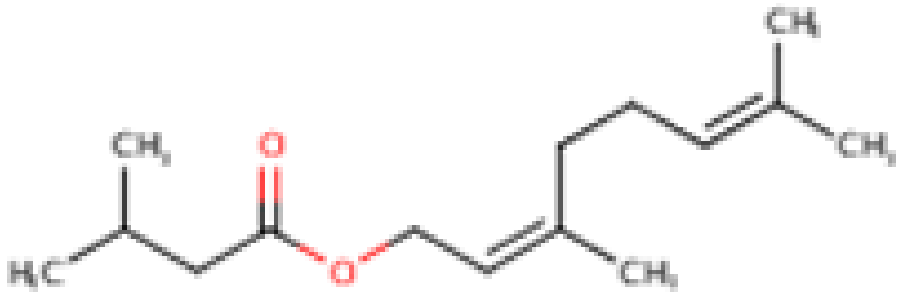
	
Molecular Formula	C14H24O2
Molecular Weight	224.34

Chemical Name in the Inventory and Synonyms	**Propanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-** Isobutyric acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-
CAS Number	2345-26-8
Structural Formula	



Molecular Formula	C14H24O2
Molecular Weight	224.34

Chemical Name in the Inventory and Synonyms	**Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (Z)-** Geranyl isovalerate, (Z)-
CAS Number	3915-83-1
Structural Formula	



Molecular Formula	C15H26O2
Molecular Weight	238.37

Chemical Name in the Inventory and Synonyms	**Butanoic acid, 3-oxo-, 3,7-dimethyl-2,6-octadienyl ester, (E)-** Acetoacetic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-
CAS Number	10032-00-5
Structural Formula	

Molecular Formula	C14H22O3
Molecular Weight	238.32

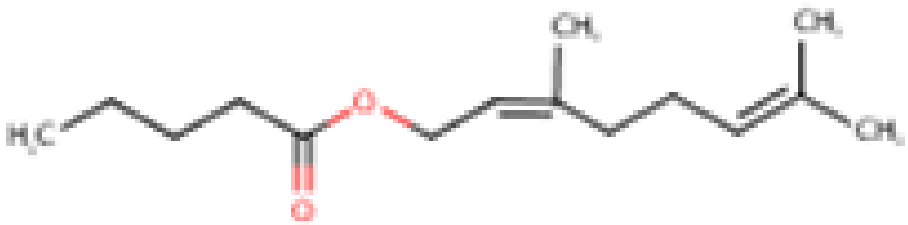
Chemical Name in the Inventory and Synonyms	**Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-** Geranyl hexanoate
CAS Number	10032-02-7
Structural Formula	

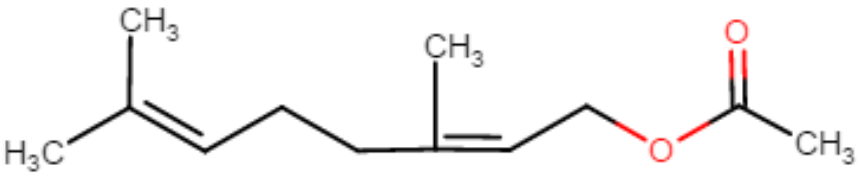
Molecular Formula	C16H28O2
Molecular Weight	252.39

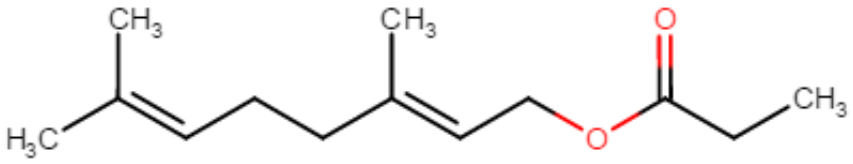
Chemical Name in the Inventory and Synonyms	**Pentanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-** Geranyl valerianate
CAS Number	10402-47-8
Structural Formula	

	
Molecular Formula	C15H26O2
Molecular Weight	238.37

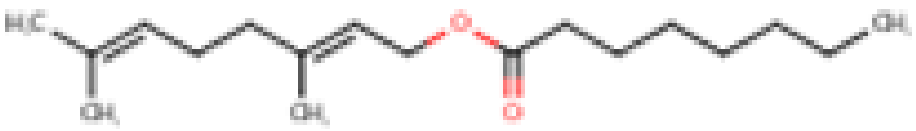
Chemical Name in the Inventory and Synonyms	**Pentanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-** 3,7-Dimethylocta-2,6-dienyl pentanoate, (Z)-
CAS Number	10522-33-5
Structural Formula	

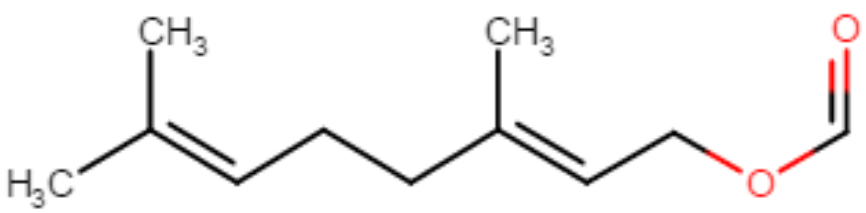
	
Molecular Formula	C15H26O2
Molecular Weight	238.37

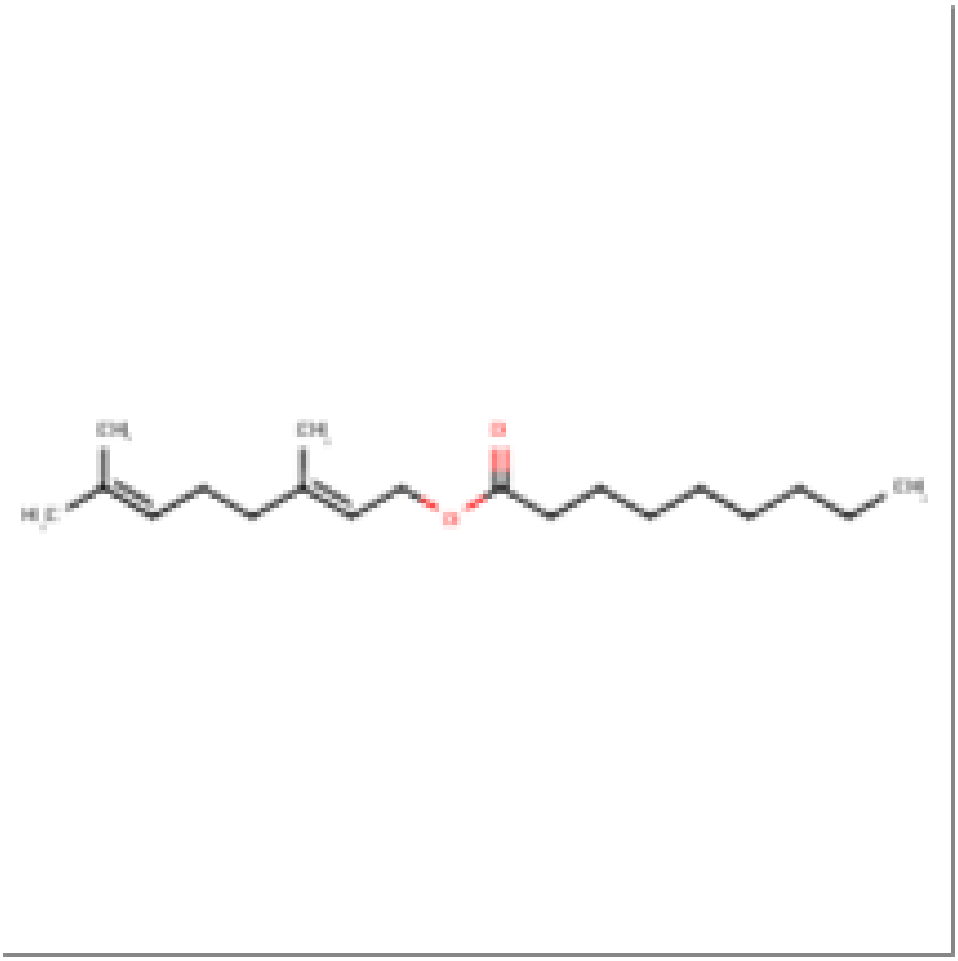
Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, acetate**
CAS Number	16409-44-2
Structural Formula	
Molecular Formula	C12H20O2
Molecular Weight	

Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate** 3,7-dimethyl-2,6-octadien-1-yl, propanoate
CAS Number	27751-90-2
Structural Formula	
Molecular Formula	C13H22O2
Molecular Weight	

Chemical Name in the Inventory and Synonyms	**Octanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-** 3,7-Dimethyl-2,6-octadienyl octanoate, trans-
CAS Number	51532-26-4
Structural Formula	

	
Molecular Formula	C18H32O2
Molecular Weight	280.45

Chemical Name in the Inventory and Synonyms	**2,6-Octadien-1-ol, 3,7-dimethyl-, formate**
CAS Number	61759-63-5
Structural Formula	
Molecular Formula	C11H18O2
Molecular Weight	

Chemical Name in the Inventory and Synonyms	**Nonanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-** Geranyl pelargonate
CAS Number	68039-29-2
Structural Formula	
Molecular Formula	C19H34O2
Molecular Weight	294.47

Chemical Name in the Inventory and Synonyms	**Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-** Neryl caproate
CAS Number	68310-59-8
Structural Formula	

	
Molecular Formula	C16H28O2
Molecular Weight	252.39

Share this page