

Geranylacetone

sc-250051

Material Safety Data Sheet



The Power is Question

Hazard Alert Code Key:

EXTREME

HIGH

MODERATE

LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

Geranylacetone

STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA



SUPPLIER

Company: Santa Cruz Biotechnology, Inc.

Address:

2145 Delaware Ave. Santa Cruz, CA 95060 United States of America

Telephone: 800.457.3801 or 831.457.3800

Emergency Tel: **CHEMWATCH: From within the US and Canada: 877-715-9305**

Emergency Tel: **From outside the US and Canada: +800 2436 2255 (1-800-CHEMCALL) or call +613 9573 3112**

PRODUCT USE

■ Intermediate: Fragrance

SYNONYMS

C13-H22-O, (CH₃)₂C=CHCH₂CH₂C(CH₃)=CHCH₂CH₂COCH₃, "trans-6, 10-dimethyl-5, 9-undecadien-2-one", trans-nerylacetone

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	0		
Body Contact:	2		
Reactivity:	1		
Chronic:	2		
			Min/Nil=0 Low=1 Moderate=2 High=3 Extreme=4



CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

May cause SENSITIZATION by skin contact.

Irritating to eyes, respiratory system and skin.

Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

■ The material has NOT been classified as "harmful by ingestion". This is because of the lack of corroborating animal or human evidence. The material may still be damaging to the health of the individual, following ingestion, especially where pre-existing organ (e.g. liver, kidney) damage is evident. Present definitions of harmful or toxic substances are generally based on doses producing mortality (death) rather than those producing morbidity (disease, ill-health). Gastrointestinal tract discomfort may produce nausea and vomiting. In an occupational setting however, unintentional ingestion is not thought to be cause for concern.

EYE

■ This material can cause eye irritation and damage in some persons.

SKIN

■ This material can cause inflammation of the skin on contact in some persons.

■ The material may accentuate any pre-existing dermatitis condition.

■ Skin contact is not thought to have harmful health effects, however the material may still produce health damage following entry through wounds, lesions or abrasions.

■ Open cuts, abraded or irritated skin should not be exposed to this material.

■ Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

■ The material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage.

■ The material has NOT been classified as "harmful by inhalation". This is because of the lack of corroborating animal or human evidence. In the absence of such evidence, care should nevertheless be taken to ensure exposure is kept to a minimum and that suitable control measures be used, in an occupational setting to control vapors, fumes and aerosols.

■ Inhalation hazard is increased at higher temperatures.

CHRONIC HEALTH EFFECTS

■ Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems. Skin contact with the material is more likely to cause a sensitization reaction in some persons compared to the general population.

Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.

In the presence of air, a number of common flavour and fragrance chemicals can form peroxides surprisingly fast. Antioxidants can in most cases minimise the oxidation.

Fragrance terpenes are generally easily oxidised in air. Non-oxidised limonene, linalool and caryophyllene turned out to be very weak sensitizers, however after oxidation limonene hydroperoxide and linalool hydroperoxide are strong sensitizers. Of the patients tested 2.6% showed positive reaction to oxidised limonene, 1.3% to oxidised linalool, 1.1% to linalool hydroperoxide, 0.5% to oxidised caryophyllene, while testing with caryophyllene oxide and oxidised myrcene resulted in few positive patch tests. 2/3 of the patients reacting positive to oxidised terpenes had fragrance related contact allergy and/or positive history for adverse reactions to fragrances.

As well as the hydroperoxides produced by linalol, limonene and delta-3-carene other oxidation and resinification effects progressively causes other fairly major changes in essential oil quality over time. Autoxidation of fragrance terpenes contributes greatly to fragrance allergy, which emphasizes the need of testing with compounds that patients are actually exposed to and not only with the ingredients originally applied in commercial formulations.

Peroxidisable terpenes and terpenoids should only be used when the level of peroxides is kept to the lowest practicable level, for instance by adding antioxidants at the time of production. Such products should have a peroxide value of less than 10 millimoles peroxide per liter. This requirement is based on the published literature mentioning sensitising properties when containing peroxides.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
geranylacetone	3796-70-1	>98
nerylacetone	3879-26-3	

Section 4 - FIRST AID MEASURES

SWALLOWED

-
- Immediately give a glass of water.
- First aid is not generally required. If in doubt, contact a Poisons Information Center or a doctor.

EYE

- If this product comes in contact with the eyes:
 - Wash out immediately with fresh running water.
 - Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.
 - If pain persists or recurs seek medical attention.
 - Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.

SKIN

- If skin contact occurs:
 - Immediately remove all contaminated clothing, including footwear
 - Flush skin and hair with running water (and soap if available).
 - Seek medical attention in event of irritation.

INHALED

-
- If fumes or combustion products are inhaled remove from contaminated area.
- Lay patient down. Keep warm and rested.
- Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures.
- Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary.
- Transport to hospital, or doctor, without delay.

NOTES TO PHYSICIAN

- Treat symptomatically.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Not available
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	0.873
Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA

-
- Foam.
- Dry chemical powder.
- BCF (where regulations permit).
- Carbon dioxide.
- Water spray or fog - Large fires only.

FIRE FIGHTING

-
- Alert Emergency Responders and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.
- Prevent, by any means available, spillage from entering drains or water course.
- Use water delivered as a fine spray to control fire and cool adjacent area.
- Avoid spraying water onto liquid pools.
- Do not approach containers suspected to be hot.
- Cool fire exposed containers with water spray from a protected location.
- If safe to do so, remove containers from path of fire.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

-
- Combustible.
- Slight fire hazard when exposed to heat or flame.
- Heating may cause expansion or decomposition leading to violent rupture of containers.
- On combustion, may emit toxic fumes of carbon monoxide (CO).
- May emit acrid smoke.
- Mists containing combustible materials may be explosive.

Combustion products include: carbon dioxide (CO₂), other pyrolysis products typical of burning organic material.

FIRE INCOMPATIBILITY

- Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids, chlorine bleaches, pool chlorine etc. as ignition may result.

PERSONAL PROTECTION

Glasses:

Chemical goggles.

Gloves:

Respirator:
Type A-P Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

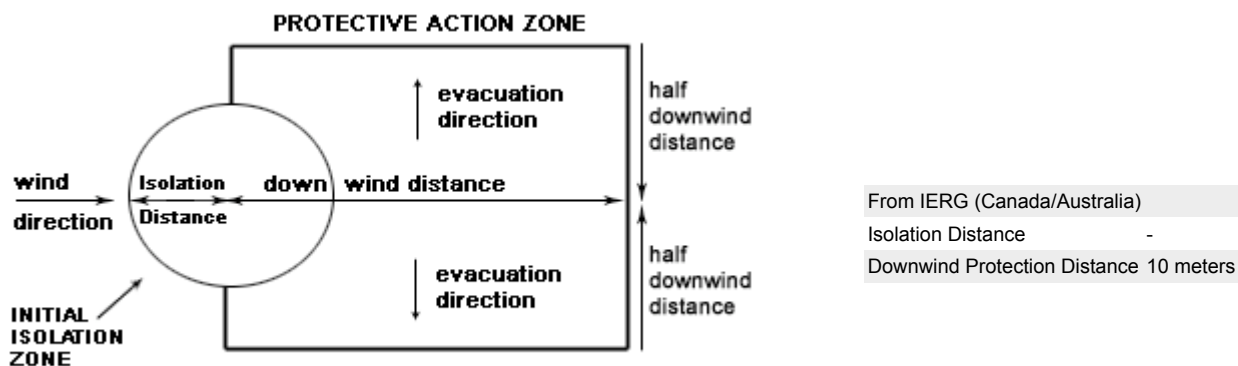
MINOR SPILLS

- Environmental hazard - contain spillage.
- Clean up all spills immediately.
- Avoid breathing vapors and contact with skin and eyes.
- Control personal contact by using protective equipment.
- Contain and absorb spill with sand, earth, inert material or vermiculite.
- Wipe up.
- Place in a suitable labeled container for waste disposal.

MAJOR SPILLS

- Environmental hazard - contain spillage.
- Moderate hazard.
- Clear area of personnel and move upwind.
- Alert Emergency Responders and tell them location and nature of hazard.
- Wear breathing apparatus plus protective gloves.
- Prevent, by any means available, spillage from entering drains or water course.
- No smoking, naked lights or ignition sources. Increase ventilation.
- Stop leak if safe to do so.
- Contain spill with sand, earth or vermiculite.
- Collect recoverable product into labeled containers for recycling.
- Absorb remaining product with sand, earth or vermiculite.
- Collect solid residues and seal in labeled drums for disposal.
- Wash area and prevent runoff into drains.
- If contamination of drains or waterways occurs, advise emergency services.

PROTECTIVE ACTIONS FOR SPILL



From US Emergency Response Guide 2000 Guide 171

FOOTNOTES

1 PROTECTIVE ACTION ZONE is defined as the area in which people are at risk of harmful exposure. This zone assumes that random changes in wind direction confines the vapour plume to an area within 30 degrees on either side of the predominant wind direction, resulting in a crosswind protective action distance equal to the downwind protective action distance.

2 PROTECTIVE ACTIONS should be initiated to the extent possible, beginning with those closest to the spill and working away from the site in the downwind direction. Within the protective action zone a level of vapour concentration may exist resulting in nearly all unprotected persons becoming incapacitated and unable to take protective action and/or incurring serious or irreversible health effects.

3 INITIAL ISOLATION ZONE is determined as an area, including upwind of the incident, within which a high probability of localised wind reversal may expose nearly all persons without appropriate protection to life-threatening concentrations of the material.

4 SMALL SPILLS involve a leaking package of 200 litres (55 US gallons) or less, such as a drum (jerrican or box with inner containers). Larger packages leaking less than 200 litres and compressed gas leaking from a small cylinder are also considered "small spills". LARGE SPILLS involve many small leaking packages or a leaking package of greater than 200 litres, such as a cargo tank, portable tank or a "one-tonne" compressed gas cylinder.

5 Guide 171 is taken from the US DOT emergency response guide book.

6 IERG information is derived from CANUTEC - Transport Canada.

ACUTE EXPOSURE GUIDELINE LEVELS (AEGL) (in ppm)

AEGL 1: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL 2: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL 3: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING



- DO NOT allow clothing wet with material to stay in contact with skin
- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- Use in a well-ventilated area.
- Prevent concentration in hollows and sumps.
- DO NOT enter confined spaces until atmosphere has been checked.
- Avoid smoking, naked lights or ignition sources.
- Avoid contact with incompatible materials.
- When handling, DO NOT eat, drink or smoke.
- Keep containers securely sealed when not in use.
- Avoid physical damage to containers.
- Always wash hands with soap and water after handling.
- Work clothes should be laundered separately.
- Use good occupational work practice.
- Observe manufacturer's storing and handling recommendations.
- Atmosphere should be regularly checked against established exposure standards to ensure safe working conditions.

RECOMMENDED STORAGE METHODS



- Metal can or drum
- Packing as recommended by manufacturer.
- Check all containers are clearly labeled and free from leaks.

STORAGE REQUIREMENTS



- Store in original containers.
- Keep containers securely sealed.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.
- Protect containers against physical damage and check regularly for leaks.
- Observe manufacturer's storing and handling recommendations.

SAFE STORAGE WITH OTHER CLASSIFIED CHEMICALS



X: Must not be stored together

O: May be stored together with specific precautions

+: May be stored together

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

The following materials had no OELs on our records

• geranylacetone: CAS:3796-70-1

• nerylacetone: CAS:3879-26-3

MATERIAL DATA

GERANYLACETONE:

NERYLACETONE:

■ Sensory irritants are chemicals that produce temporary and undesirable side-effects on the eyes, nose or throat. Historically occupational

exposure standards for these irritants have been based on observation of workers' responses to various airborne concentrations. Present day expectations require that nearly every individual should be protected against even minor sensory irritation and exposure standards are established using uncertainty factors or safety factors of 5 to 10 or more. On occasion animal no-observable-effect-levels (NOEL) are used to determine these limits where human results are unavailable. An additional approach, typically used by the TLV committee (USA) in determining respiratory standards for this group of chemicals, has been to assign ceiling values (TLV C) to rapidly acting irritants and to assign short-term exposure limits (TLV STELs) when the weight of evidence from irritation, bioaccumulation and other endpoints combine to warrant such a limit. In contrast the MAK Commission (Germany) uses a five-category system based on intensive odour, local irritation, and elimination half-life. However this system is being replaced to be consistent with the European Union (EU) Scientific Committee for Occupational Exposure Limits (SCOEL); this is more closely allied to that of the USA.

OSHA (USA) concluded that exposure to sensory irritants can:

- cause inflammation
- cause increased susceptibility to other irritants and infectious agents
- lead to permanent injury or dysfunction
- permit greater absorption of hazardous substances and
- acclimate the worker to the irritant warning properties of these substances thus increasing the risk of overexposure.

PERSONAL PROTECTION



Consult your EHS staff for recommendations

EYE

-
- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses pose a special hazard; soft lenses may absorb irritants and all lenses concentrate them. DO NOT wear contact lenses.

HANDS/FEET

■ Wear chemical protective gloves, eg. PVC.

Wear safety footwear or safety gumboots, eg. Rubber.

NOTE: The material may produce skin sensitization in predisposed individuals. Care must be taken, when removing gloves and other protective equipment, to avoid all possible skin contact.

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include: such as:

- frequency and duration of contact,
- chemical resistance of glove material,
- glove thickness and
- dexterity

Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).

- When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.
- When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.
- Contaminated gloves should be replaced.

Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

- Neoprene gloves

OTHER

-
- Overalls.
- P.V.C. apron.
- Barrier cream.
- Skin cleansing cream.
- Eye wash unit.

RESPIRATOR

■ Selection of the Class and Type of respirator will depend upon the level of breathing zone contaminant and the chemical nature of the contaminant. Protection Factors (defined as the ratio of contaminant outside and inside the mask) may also be important.

Breathing Zone Level ppm (volume)	Maximum Protection Factor	Half-face Respirator	Full-Face Respirator
1000	10	A-1 P	-
1000	50	-	A-1 P
5000	50	Airline*	-
5000	100	-	A-2 P
10000	100	-	A-3 P
	100+		Airline* *

* - Continuous Flow ** - Continuous-flow or positive pressure demand.

The local concentration of material, quantity and conditions of use determine the type of personal protective equipment required.

Use appropriate NIOSH-certified respirator based on informed professional judgement. In conditions where no reasonable estimate of exposure can be made, assume the exposure is in a concentration IDLH and use NIOSH-certified full face pressure demand SCBA with a minimum service life of 30 minutes, or a combination full facepiece pressure demand SAR with auxiliary self-contained air supply. Respirators provided only for escape from IDLH atmospheres shall be NIOSH-certified for escape from the atmosphere in which they will be used.

ENGINEERING CONTROLS

■ Local exhaust ventilation usually required. If risk of overexposure exists, wear an approved respirator. Correct fit is essential to obtain adequate protection an approved self contained breathing apparatus (SCBA) may be required in some situations. Provide adequate ventilation in warehouse or closed storage area.

Air contaminants generated in the workplace possess varying "escape" velocities which, in turn, determine the "capture velocities" of fresh circulating air required to effectively remove the contaminant.

Type of Contaminant:	Air Speed:
solvent, vapors, degreasing etc., evaporating from tank (in still air).	0.25-0.5 m/s (50-100 f/min.)
aerosols, fumes from pouring operations, intermittent container filling, low speed conveyer transfers, welding, spray drift, plating acid fumes, pickling (released at low velocity into zone of active generation)	0.5-1 m/s (100-200 f/min.)
direct spray, spray painting in shallow booths, drum filling, conveyer loading, crusher dusts, gas discharge (active generation into zone of rapid air motion)	1-2.5 m/s (200-500 f/min.)
grinding, abrasive blasting, tumbling, high speed wheel generated dusts (released at high initial velocity into zone of very high rapid air motion).	2.5-10 m/s (500-2000 f/min.)

Within each range the appropriate value depends on:

Lower end of the range	Upper end of the range
1: Room air currents minimal or favorable to capture	1: Disturbing room air currents
2: Contaminants of low toxicity or of nuisance value only.	2: Contaminants of high toxicity
3: Intermittent, low production.	3: High production, heavy use
4: Large hood or large air mass in motion	4: Small hood-local control only

Simple theory shows that air velocity falls rapidly with distance away from the opening of a simple extraction pipe. Velocity generally decreases with the square of distance from the extraction point (in simple cases). Therefore the air speed at the extraction point should be adjusted, accordingly, after reference to distance from the contaminating source. The air velocity at the extraction fan, for example, should be a minimum of 1-2 m/s (200-400 f/min) for extraction of solvents generated in a tank 2 meters distant from the extraction point. Other mechanical considerations, producing performance deficits within the extraction apparatus, make it essential that theoretical air velocities are multiplied by factors of 10 or more when extraction systems are installed or used.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Liquid.

Does not mix with water.

Floats on water.

State	Liquid	Molecular Weight	194.32
Melting Range (°F)	Not available	Viscosity	Not Available
Boiling Range (°F)	255.2 (10 mm Hg)	Solubility in water (g/L)	Partly miscible
Flash Point (°F)	>230	pH (1% solution)	Not applicable.
Decomposition Temp (°F)	Not available.	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapour Pressure (mmHG)	Not available
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	0.873
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	>1
Volatile Component (%vol)	Not available	Evaporation Rate	Not available

APPEARANCE

Liquid; does not mix well with water.

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

■

- Presence of incompatible materials.

- Product is considered stable.
- Hazardous polymerization will not occur.

STORAGE INCOMPATIBILITY



- Avoid strong bases.

Avoid reaction with oxidizing agents.

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

GERANYLACETONE

TOXICITY AND IRRITATION

■ unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

■ Contact allergies quickly manifest themselves as contact eczema, more rarely as urticaria or Quincke's edema. The pathogenesis of contact eczema involves a cell-mediated (T lymphocytes) immune reaction of the delayed type. Other allergic skin reactions, e.g. contact urticaria, involve antibody-mediated immune reactions. The significance of the contact allergen is not simply determined by its sensitization potential: the distribution of the substance and the opportunities for contact with it are equally important. A weakly sensitizing substance which is widely distributed can be a more important allergen than one with stronger sensitizing potential with which few individuals come into contact. From a clinical point of view, substances are noteworthy if they produce an allergic test reaction in more than 1% of the persons tested.

Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound. Key criteria for the diagnosis of RADS include the absence of preceding respiratory disease, in a non-atopic individual, with abrupt onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. A reversible airflow pattern, on spirometry, with the presence of moderate to severe bronchial hyperreactivity on methacholine challenge testing and the lack of minimal lymphocytic inflammation, without eosinophilia, have also been included in the criteria for diagnosis of RADS. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. Industrial bronchitis, on the other hand, is a disorder that occurs as result of exposure due to high concentrations of irritating substance (often particulate in nature) and is completely reversible after exposure ceases. The disorder is characterised by dyspnea, cough and mucus production.

For terpenoid primary alcohols and related esters

This family includes three terpenoid acyclic aliphatic primary alcohols, citronellol, geraniol, and nerol. The category also includes a mixture of terpenoid esters and alcohols called acetylated myrcene. Geranyl acetate and neryl acetate are the principal products formed when myrcene is acetylated. Thus, the mixture is commonly recognised as acetylated myrcene. The four substances are grouped together because of their close structural relationships and the resulting similarities of their physicochemical and toxicological properties. Citronellol, geraniol, nerol, and geranyl acetate are currently recognized by the U.S. Food and Drug Administration (FDA) as GRAS ("generally regarded as safe") for their intended use as flavouring substances

In nature, terpenes are produced by the isoprene pathway that is an integral part of normal plant and animal biosynthesis. Oxygenated terpene substances {e.g., geraniol, nerol, citronellol, citral (a mixture of aldehydes, geranial and neral), and geranyl acetate} are therefore, ubiquitous in the plant kingdom

Acetylated myrcene (geranyl and neryl acetate), being mainly a mixture of esters, is expected to be somewhat less polar and therefore less water soluble than the three terpenoid alcohols. It is however, expected to be rapidly hydrolysed in vivo to yield nerol, geraniol, and acetic acid. Similar hydrolysis also occurs in the environment albeit at a somewhat slower rate. Terpenoid alcohols formed in the gastrointestinal tract, as a result of hydrolysis are rapidly absorbed.

Following hydrolysis, geraniol, nerol, and citronellol undergo a complex pattern of alcohol oxidation, omega-oxidation, hydration, selective hydrogenation and subsequent conjugation to form oxygenated polar metabolites, which are rapidly excreted primarily in the urine of animals. Alternately, the corresponding carboxylic acids formed by oxidation of the alcohol function may enter the beta-oxidation pathway and eventually undergo cleavage to yield shorter chain carboxylic acids that are completely metabolised to carbon dioxide. Geraniol, related terpenoid alcohols (citronellol and nerol), and the related terpene aldehydes (geranial and neral) exhibit similar pathways of metabolic detoxication in animals.

In rats and mice, a mixture of geranial and neral, commonly recognised as citral, undergoes rapid absorption from the gastrointestinal tract and distribution throughout the body.

Genotoxicity: In vitro genotoxicity assays available for citronellol, geraniol, citral (geranial and neral mixture) and acetylated myrcene (geranyl acetate and neryl acetate mixture) demonstrate that these substances have a low genotoxic potential. No evidence of mutagenicity was reported in an Ames assay with citronellol metabolites. In two chromosomal aberration assays with geraniol and a geranial/neral mixture, there was no evidence of increased incidence of chromosomal aberrations when Chinese hamster lung fibroblasts were incubated with 125 ug/plate of geraniol or 30 ug/plate of the geranial/neral mixture, respectively. Nerol, being a geometrical isomer of geraniol would also be expected to be negative. The acetates of nerol and geraniol, the principal constituents of acetylated myrcene, which will hydrolyse to nerol and geraniol, have also been tested and found to be negative in Ames assays at concentrations up to 20,000 ug/plate.

In vivo: Tests on citronellol and acetylated myrcene (geranyl acetate) confirm the lack of genotoxic potential. A mixture of geranyl acetate (79%) and citronellyl acetate (21%) showed no evidence of increased micronuclei in a standardized mouse (B6C3F1 strain) micronucleus assay at dose levels up to and including 1800 mg/kg bw and there was no evidence of unscheduled DNA synthesis when the geranyl acetate/citronellyl acetate mixture was given orally to Fisher F344 rats. Since these esters hydrolyse to geraniol and citronellol in rodents, these results apply directly to geraniol and citronellol.

Repeat dose toxicity:

Short term: Citronellol, as an equal mixture with the structurally similar material linalool, administered to rats at 100 mg/kg/day for 12 weeks, resulted in no adverse effects. Geraniol, in combination with a structural isomer, was administered to groups of rats (5/sex/group) in the diet at concentrations of 10,000 ppm for 16 weeks or 1000 ppm for 27 weeks. No adverse effects were reported in either study. Likewise, no adverse effects were observed when rats were maintained on a diet calculated to provide an estimated average daily intake of greater than 200 mg/kg bw/day of citral, a mixture of geranial and neral, for 91 days.

Long-term studies: Citronellol, geraniol and nerol and the principal hydrolysis products of acetylated myrcene (geranyl acetate) were all included as structural similar acyclic terpenes in a QSAR study by molecular orbital calculations for prediction of their potential toxicity/carcinogenicity. None of the substances in this group were predicted to have significant toxicity and/or carcinogenicity potential. This conclusion is supported by the results of a 2 year bioassay on a mixture of acetate esters of geraniol and citronellol that showed no toxic or carcinogenic effects at dose levels up to 2000 mg/kg bw/day in rats and 1000 mg/kg bw/day in mice.

Reproductive toxicity: A mixture of the aldehydes, geranial and neral, has been subjected to an oral 2-generation reproductive study in rats. There were no reproductive effects at the maternal NOAEL of 50 mg/kg/day and a foetal/pup NOAEL of 160 mg/kg bw/day. At a maternally toxic level of 500 mg/kg bw/day, the only effect reported was a slightly decreased pup weight. Given that other studies show the mixture of aldehydes exhibits a higher level of toxicity than the corresponding alcohols geraniol and nerol, data on reproductive and developmental toxicity for the aldehydes may be used to conservatively estimate reproductive toxicity for the corresponding alcohols.

Developmental toxicity: In a developmental/reproduction screening study, rats were administered the acetal formed from citral (geranial and neral mixture) and ethanol. The acetal will readily hydrolyse to citral. The NOAELs for maternal toxicity and developmental toxicity were reported to be 125 and 250 mg/kg bw/day, respectively.

A geranial/neral mixture has been subjected to an oral foetotoxicity study in rats an NOAEL for maternal and developmental toxicities were reported to be 60 mg/kg bw/day

In an inhalation developmental study in rats using a geranial/ neral mixture A NOAEL for maternal toxicity was reported to be 35 ppm. There were some slight foetotoxic effects at the maternally toxic level of 85 ppm (as a vapor/aerosol).

No significant acute toxicological data identified in literature search.

Section 12 - ECOLOGICAL INFORMATION

Refer to data for ingredients, which follows:

NERYLACETONE:

GERANYLACETONE:

■ DO NOT discharge into sewer or waterways.

■ Terpenes such as limonene and isoprene contribute to aerosol and photochemical smog formation. Emissions of biogenic hydrocarbons, such as the terpenes, to the atmosphere may either decrease ozone concentrations when oxides of nitrogen are low or, if emissions take place in polluted air (i.e containing high concentrations of nitrogen oxides), leads to an increase in ozone concentrations. Lower terpenoids can react with unstable reactive gases and may act as precursors of photochemical smog therefore indirectly influencing community and ecosystem properties.

Complex chlorinated terpenes such as toxaphene (a persistent, mobile and toxic insecticide) and its degradation products, were produced by photoinitiated reactions in an aqueous system, initially containing limonene and other monoterpenes, simulating pulp bleach conditions

The reactions of ozone with larger unsaturated compounds, such as the terpenes can give rise to oxygenated species with low vapour pressures that subsequently condense to form secondary organic aerosol.

GERANYLACETONE:

Marine Pollutant:	Yes
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■ Toxic to aquatic organisms.

■ Do NOT allow product to come in contact with surface waters or to intertidal areas below the mean high water mark. Do not contaminate water when cleaning equipment or disposing of equipment wash-waters.

Wastes resulting from use of the product must be disposed of on site or at approved waste sites.

■ May cause long-term adverse effects in the aquatic environment.

■ For terpenoid primary alcohols and related esters

Environmental fate:

Water solubility: While the reported water solubilities were not obtained according to OECD guidelines, the agreement of the values reported, 600 mg/L for citronellol and 300 mg/L for geraniol, with the calculated values 211, 256 and 256 mg/L for citronellol, geraniol and nerol, respectively, support their reliability. No water solubility data are available for acetylated myrcene. However, the principle components being esters have lower solubilities than their component alcohols. The calculated water solubilities of neryl acetate and geranyl acetate are both 6.9 mg/L. The other major component, limen has a calculated solubility of 3.1 mg/L.

Photodegradation: The calculated photodegradation half lives for citronellol, geraniol and nerol are in the range from 19 minutes to 1.3 hours. Acetylated myrcene can be expected to be in the same range since the calculated half-life for its principal constituents, neryl acetate and geranyl acetate, is 19 minutes and for the second major constituent, limen, is 37 minutes. Structurally, these substances are unsaturated primary alcohols that have the potential to form radical species in the gas phase and also be oxidized to the corresponding unsaturated aldehyde. The known chemical reactivity of these substrates supports short photodegradation half-lives predicted by the model.

Stability in Water: No hydrolysis is possible for the three terpenoid primary alcohols, citronellol, geraniol and nerol. All three are expected to be very stable in aqueous solution. The principal constituents of acetylated myrcene, geranyl acetate and neryl acetate are esters and are calculated to have half-lives for hydrolysis of 23 days at pH 8 and 231 days at pH 7. Hydrolysis of geranyl acetate and neryl acetate is expected both in vivo and in the environment. The second major constituent of acetylated myrcene, limen, will not hydrolyse in water. The significance of calculated half-life data for geranyl acetate must take into account the experimental data that aliphatic ester, in general, are readily hydrolysed in fish.

Biodegradation: Duplicate studies on citronellol and geraniol show these materials to be readily biodegradable (i.e., 100% biodegradation [OECD 301B, OECD 301C]. Likewise, a mixture of geranial and neral (citral) exhibits greater than 92% and 99.5% biodegradation. Nerol is a stereoisomer of geraniol and would likewise be expected to be readily biodegradable. Geranyl acetate has also been shown to be readily biodegradable (greater than 82% biodegradation) and, therefore, neryl acetate would be as well. The other significant constituent of acetylated myrcene, limen, has not been shown to be readily biodegradable. However, since limen makes up only 10% of the mixture, a ready biodegradation test of the mixture is expected to result in apparent ready biodegradation. In summary, all members of the chemical category are expected to readily biodegrade in the environment.

Ecotoxicity:

Experimental data for citronellol, geraniol, nerol, and citral indicates a very low order of acute toxicity to algae. No inhibition to growth was observed at 100 mg/L for any of the four substances.

NERYLACETONE:

Ecotoxicity

Ingredient
geranylacetone
nerylacetone

Persistence: Water/Soil
HIGH
HIGH

Persistence: Air

Bioaccumulation
LOW
LOW

Mobility
MED
MED

Section 13 - DISPOSAL CONSIDERATIONS

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

! Puncture containers to prevent re-use and bury at an authorized landfill.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction
- Reuse
- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.

DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.

- Recycle wherever possible or consult manufacturer for recycling options.
- Consult Waste Management Authority for disposal.
- Bury or incinerate residue at an approved site.
- Recycle containers if possible, or dispose of in an authorized landfill.

Section 14 - TRANSPORTATION INFORMATION



DOT:

Symbols:	G	Hazard class or Division:	9
Identification Numbers:	UN3082	PG:	III
Label Codes:	9	Special provisions:	8, 146, 335, IB3, T4, TP1, TP29
Packaging: Exceptions:	155	Packaging: Non-bulk:	203
Packaging: Exceptions:	155	Quantity limitations: Passenger aircraft/rail:	No limit
Quantity Limitations: Cargo aircraft only:	No limit	Vessel stowage: Location:	A
Vessel stowage: Other:	None		

Hazardous materials descriptions and proper shipping names:

Environmentally hazardous substance, liquid, n.o.s

Air Transport IATA:

ICAO/IATA Class:	9	ICAO/IATA Subrisk:	None
UN/ID Number:	3082	Packing Group:	III
Special provisions:	A97		

Shipping Name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. *(CONTAINS GERANYLACETONE)

Maritime Transport IMDG:

IMDG Class:	9	IMDG Subrisk:	None
UN Number:	3082	Packing Group:	III
EMS Number:	F-A , S-F	Special provisions:	179 274 335 909
Limited Quantities:	5 L	Marine Pollutant:	Yes

Shipping Name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.(contains geranylacetone)

Section 15 - REGULATORY INFORMATION



REGULATIONS

geranylacetone (CAS: 3796-70-1) is found on the following regulatory lists;

"Canada Domestic Substances List (DSL)", "US Food Additive Database", "US Toxic Substances Control Act (TSCA) - Inventory"

Regulations for ingredients

No data for nerylacetone (CAS: , 3879-26-3)

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

■ Cumulative effects may result following exposure*.

* (limited evidence).

Denmark Advisory list for selfclassification of dangerous substances

Substance	CAS	Suggested codes
nerylacetone	3879- 26- 3	N R51/53

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■ Classification of the mixture and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

A list of reference resources used to assist the committee may be found at:
www.chemwatch.net/references.

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

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