β-Damascenone

sc-218066

Material Safety Data Sheet

The Power to Question

Hazard Alert Code Key: EXTREME | HIGH | MODERATE | LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

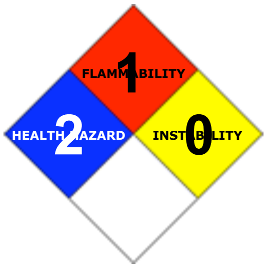
PRODUCT NAME

β-Damascenone

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
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

- In perfumery/ flavouring. Fragrance

SYNONYMS

C13-H20-O, "(Z)-1-(2, 6, 6-trimethyl-1-cyclohex-2-enyl)but-2-en-", 1-one, "1-trimethyl-2-cyclohexen-1-(2, 6, 6-yl)-2-butenone", 4-trimethyl-2-cyclohexenyl)-2-buten-4-one, "4-(2, 6, 6-trimethyl-2-cyclohexenyl-1)-2-buten-4-one", "2-buten-1-on, 1-(2, 6, 6-trimethyl-1, 3-cyclohexadien-1-yl)-, (Z)-", (Z)-damascenone, cis-damascenone, cis-beta-damascenone, "2-buten-1-one, 1-(2, 6, 6-trimethyl-3-cyclohexen-1-yl)-, ", Damarose-alpha, "Dihydrofloriffone A"

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	2		
Body Contact:	2		
Reactivity:	2		

Min/Nil=0
Low=1
Moderate=2
High=3
Extreme=4

Chronic: 2

CANADIAN WHMIS SYMBOLS

EMERGENCY OVERVIEW

RISK

Explosive when dry.
May cause SENSITIZATION by skin contact.
Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

- Accidental ingestion of the material may be damaging to the health of the individual.

EYE

- Although the liquid is not thought to be an irritant, direct contact with the eye may produce transient discomfort characterized by tearing or conjunctival redness (as with windburn).

SKIN

- The liquid may be miscible with fats or oils and may degrease the skin, producing a skin reaction described as non-allergic contact dermatitis. The material is unlikely to produce an irritant dermatitis as described in EC Directives .
- 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

- Inhalation of vapours may cause drowsiness and dizziness. This may be accompanied by narcosis, reduced alertness, loss of reflexes, lack of coordination and vertigo.
- There is some evidence to suggest that the material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage.
- Inhalation hazard is increased at higher temperatures.
- Inhalation of high concentrations of gas/vapor causes lung irritation with coughing and nausea, central nervous depression with headache and dizziness, slowing of reflexes, fatigue and inco-ordination.

CHRONIC HEALTH EFFECTS

- Skin contact with the material is more likely to cause a sensitization reaction in some persons compared to the general population.

There is some evidence that inhaling this product is more likely to cause a sensitization reaction in some persons compared to the general population.

Certain substances, commonly found in perfumes or perfumed products, produce hypersensitivity. Sensitising constituents have been classified as Class A (common sensitisers) or Class B (rare sensitisers) in a Japanese study (Nakayama 1998). Contact allergy to perfumes occurs with a relatively high incidence, such incidence only surpassed by nickel allergy in the community. In a Danish study, it was found that about 1.1% of the population was allergic to Peru balsam or "fragrance mix".

There is no cure for perfume allergy. Once sensitised, exposure to even minute amounts of the perfume, gives rise to eruptions and eczema. These symptoms may be treated with steroid creams, although frequent recourse to this treatment produces unwanted side-effects.

Orally administered ionones and structurally related substances are absorbed and metabolized in mammals by allylic hydroxylation of the ring followed by oxidation of the hydroxyl group to 3-oxo derivatives. Reduction of the ketone function to the corresponding secondary alcohol also occurs. Combinations of these detoxication reactions result in the formation of multiple polar metabolites, which are excreted in the urine unchanged or conjugated with glucuronic acid.

The metabolism of ionones is expected to be similar in humans. This is supported by human metabolism studies of retinoids and carotenoids such as cis-13-retinoic acid (i.e., isotretinoin) and beta-carotene, respectively, which possess ionone fragments. The primary blood and biliary metabolites following oral administration of isotretinoin to humans include the glucuronic acid conjugates of isotretinoin and the allylic oxidation product.

Rat oral LD50 values available for alpha-ionone, alpha-iso-methylionone, methylionone (mixture of isomers), and gamma-ionone indicate these materials to be very low in oral acute toxicity. The LD50 values of all four substances are greater than 5000 mg/kg bw. Mouse oral LD50 values are also greater than 5000 mg/kg bw for alpha-ionone, alpha-iso-methylionone, and methyl ionone (mixture of isomers). The mouse oral LD50s are reported to be 6650 mg/kg bw for alpha-ionone, 5331 mg/kg bw for methylionone, and 8714 for alpha-isomethylionone. The acute dermal LD50s reported for alpha-iso-methylionone, methylionone (mixture of isomers), and gamma-ionone are all greater than 5000 mg/kg bw. Based on these results the acute oral and dermal toxicities of ionone derivatives is concluded to be very low.

Based on the results of dietary studies with alpha-iso-methylionone, alpha-ionone, and beta-ionone and a dermal study with gamma-methylionone, it is concluded that none of the ionone derivatives exhibits any evidence of toxicity at dose levels up to and including 10 mg/kg bw/day.

The lack of reproductive toxicity is supported by observations made in three separate repeat dose studies in which there was no evidence (organ weight, gross or histopathological) toxicity to reproductive organs (testis, seminal vesicles, ovaries) of rats maintained on diets of up to 100 mg/kg bw/day for 90 days. Therefore, it is concluded that none of the ionone derivatives discussed show any evidence of reproductive toxicity.

Vitamin A (retinoid) produces teratogenicity; ionones may cleave from retinoids after oxidation. Studies of ionones indicate they are not teratogenic. The results of studies on numerous compounds indicate that teratogenic potential is associated with specific structural features in the Vitamin A which is not shared with ionones

Based on the results of this in vivo genotoxicity assays and the lack of any evidence of genotoxicity for numerous in vitro assays with and without metabolic activation, it is unlikely that any of these materials would exhibit a significant genotoxic potential in vivo.

Intolerance to perfumes, by inhalation, may occur if the perfume contains a sensitising principal. Symptoms may vary from general illness, coughing, phlegm, wheezing, chest-tightness, headache, exertional dyspnoea, acute respiratory illness, hayfever, and other respiratory diseases (including asthma). Perfumes can induce hyper-reactivity of the respiratory tract without producing an IgE-mediated allergy or demonstrable respiratory obstruction. This was shown by placebo-controlled challenges of nine patients to "perfume mix". The same patients were also subject to perfume provocation, with or without a carbon filter mask, to ascertain whether breathing through a filter with active carbon would prevent symptoms. The patients breathed through the mouth, during the provocations, as a nose clamp was used to prevent nasal inhalation. The patient's earlier symptoms were verified; breathing through the carbon filter had no protective effect. The symptoms were not transmitted via the olfactory nerve but they may have been induced by trigeminal reflex via the respiratory tract or by the eyes.

Cases of occupational asthma induced by perfume substances such as isoamyl acetate, limonene, cinnamaldehyde and benzaldehyde, tend to give persistent symptoms even though the exposure is below occupational exposure limits.

Inhalation intolerance has also been produced in animals. The emissions of five fragrance products, for one hour, produced various combinations of sensory irritation, pulmonary irritation, decreases in expiratory airflow velocity as well as alterations of the functional observational battery indicative of neurotoxicity in mice. Neurotoxicity was found to be more severe after mice were repeatedly exposed to the fragrance products, being four brands of cologne and one brand of toilet water.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
alpha-damascone	23726-93-4	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

■

- If swallowed do NOT induce vomiting.
- If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.
- Observe the patient carefully.
- Never give liquid to a person showing signs of being sleepy or with reduced awareness; i.e. becoming unconscious.
- Give water to rinse out mouth, then provide liquid slowly and as much as casualty can comfortably drink.
- Seek medical advice.

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.
- Other measures are usually unnecessary.

NOTES TO PHYSICIAN

■ Treat symptomatically.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Not Available
Upper Explosive Limit (%):	Not Available
Specific Gravity (water=1):	0.89
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 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.

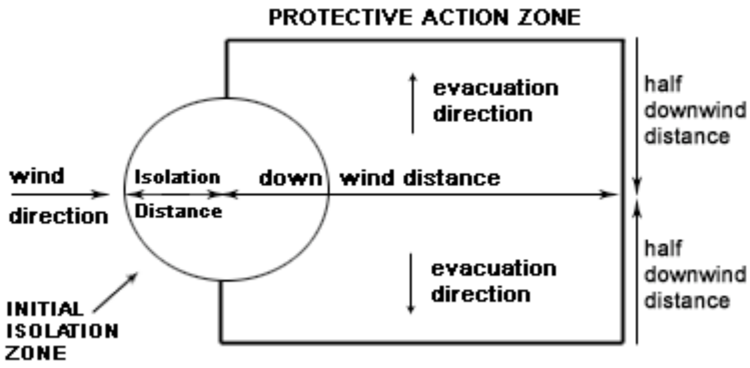
MAJOR SPILLS

■ 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 IERG (Canada/Australia)	
Isolation Distance	-
Downwind Protection Distance	10 meters

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 + X X +

X: Must not be stored together
O: May be stored together with specific preventions
+: May be stored together

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m³	STEL ppm	STEL mg/m³	Peak ppm	Peak mg/m³	TWA F/CC	Notes
Canada - Alberta Occupational Exposure Limits	alpha-damascone (Turpentine and selected monoterpenes)	20	111						

MATERIAL DATA

ALPHA-DAMASCONE:

■ 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.

Class A fragrance - common cosmetic and primary sensitizer (Nakayama 1998).
for structural analogue beta-damascone

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	-
1000	50	-	A-1
5000	50	Airline*	-
5000	100	-	A-2
10000	100	-	A-3
	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.

State	Liquid	Molecular Weight	192.3
Melting Range (°F)	Not Available	Viscosity	Not Available
Boiling Range (°F)	Not Available	Solubility in water (g/L)	Partly Miscible
Flash Point (°F)	>199.4	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)	0.89
Lower Explosive Limit (%)	Not Available	Relative Vapor Density (air=1)	Not Available
Volatile Component (%vol)	Not Available	Evaporation Rate	Not Available

APPEARANCE

Light-yellow liquid with fragrant odour; does not mix well with water. Miscible with absolute alcohol.

The colorless to yellowish liquid beta-ionone has a water solubility of about 0.169 g/l and a vapor pressure of about 0.009 hPa at 25 C. The measured log Kow of 4.0 at 25 C, the calculated log Koc of 2.80 - 3.34 and the calculated BCF of 501 indicate a potential for bio- and geoaccumulation. According to distribution modeling using Mackay Level I, water (34 %), soil (27 %), sediment (27 %) and air (12 %) are the main targets for the compound. beta-Ionone is with > 70 % (within 28 days, 10-day-window criteria fulfilled) readily biodegradable according to OECD criteria. In the atmosphere, it will be rapidly photodegraded by reactions with OH radicals (calculated t1/2 1.6 hours) and ozone (calculated t1/2: 18 minutes).

Material	Value

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

■

- Presence of incompatible materials.
- Product is considered stable.
- Hazardous polymerization will not occur.

STORAGE INCOMPATIBILITY

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- The various oxides of nitrogen and peroxyacids may be dangerously reactive in the presence of alkenes. BRETHERICK L.: Handbook of Reactive Chemical Hazards
- Avoid reaction with strong Lewis or mineral acids.
- Reaction with halogens requires carefully controlled conditions.
- Free radical initiators should be avoided.

The interaction of alkenes and alkynes with nitrogen oxides and oxygen may produce explosive addition products; these may form at very low temperatures and explode on heating to higher temperatures (the addition products from 1,3-butadiene and cyclopentadiene form rapidly at -150 C and ignite or explode on warming to -35 to -15 C). These derivatives ("pseudo- nitrosites") were formerly used to characterize terpene hydrocarbons. Exposure to air must be kept to a minimum so as to limit the build-up of peroxides which will concentrate in bottoms if the product is distilled. The product must not be distilled to dryness if the peroxide concentration is substantially above 10 ppm (as active oxygen) since explosive decomposition may occur. Distillate must be immediately inhibited to prevent peroxide formation. The effectiveness of the antioxidant is limited once the peroxide levels exceed 10 ppm as active oxygen. Addition of more inhibitor at this point is generally ineffective. Prior to distillation it is recommended that the product should be washed with aqueous ferrous ammonium sulfate to destroy peroxides; the washed product should be immediately re-inhibited. A range of exothermic decomposition energies for double bonds is given as 40-90 kJ/mol. The relationship between energy of decomposition and processing hazards has been the subject of discussion; it is suggested that values of energy released per unit of mass, rather than on a molar basis (J/g) be used in the assessment. For example, in "open vessel processes" (with man-hole size openings, in an industrial setting), substances with exothermic decomposition energies below 500 J/g are unlikely to present a danger, whilst those in "closed vessel processes" (opening is a safety valve or bursting disk) present some danger where the decomposition energy exceeds 150 J/g. BRETHERICK: Handbook of Reactive Chemical Hazards, 4th Edition.
Avoid reaction with oxidizing agents.

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

Section 11 - TOXICOLOGICAL INFORMATION

ALPHA-DAMASCONE

TOXICITY AND IRRITATION

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

TOXICITY	IRRITATION
Oral (mouse) LD50: 1821 mg/kg	Nil Reported

■ 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.
No significant acute toxicological data identified in literature search.
Should not be used as fragrance ingredients such that the total level in finished cosmetic products exceeds 0.02%, individually or in combination with other isomers of damascone. Based on test data showing sensitising potential for this material and on evidence of cross-reactivity. (IFRA guidelines).

For ionone, damascones and other other structurally related compounds:

Human Health: The only hazards identified are slight irritation to the eyes and changes in the liver, kidneys and thyroid after repeated oral exposure, which were either of minor severity or were considered to be a species-specific effect in male rats ß-Ionone has only low acute toxicity after oral ingestion.
From animal experiments it can be concluded that beta-ionone is absorbed after oral exposure. Metabolism takes place mainly in the liver. Metabolites, which were identified in the urine of exposed rabbits, are 3-oxo-beta-ionone, 3-oxo-beta-ionol, dihydro-3-oxo-beta-ionol and 3-hydroxy-beta-ionol. beta-Ionone was found to be an inducer of CYP 1A and 2B isozymes in the liver of rodents.
A gavage study conducted with a mixture of 60 % a-Ionone and 40 % beta-ionone revealed a LD50 of 4590 mg/kg bw. Clinical signs of toxicity were depression and tremors. In studies conducted according to OECD test guidelines and under GLP conditions, beta-ionone was not irritating to the skin of rabbits after semiocclusive application for 4 hours and only slightly irritating to the eyes. After a 24-hours exposure under occlusive conditions, a slight irritation of the skin was observed in rabbits. A limited human patch test did not reveal a potential for skin irritation when a not further specified mixture of alpha-- and beta-ionone was applied undiluted to the skin of volunteers. A limited Guinea pig maximization test found no evidence that beta-ionone is a dermal sensitiser. According to secondary sources, ionone (a not further specified mixture of alpha-- and beta-ionone) was negative in an open epicutaneous test with Guinea pigs as well as in a human maximization test with a product containing 97.5 % alpha-ionone and 2.5 % beta-ionone.
The administration of beta-ionone over a period of 90 days according to OECD TG 408 at dietary concentrations of 100, 1000 and 10 000 ppm (7 and 8 mg/kg bw/day, 72 and 83 mg/kg bw/day or 720 and 801 mg/kg bw/day for males and females) to rats led to signs of general systemic toxicity at the high and mid dose. Target organs were liver, kidneys and thyroid glands. The liver findings in both sexes and the increased kidney weights in high dose females were indicative of adaptive and most likely reversible processes with the aim to increase the metabolizing and/or excretory capacity of these organs. The findings in males with respect to kidneys as well as kidney relevant parameters should be seen in the light of high amounts of alpha2u-globulin in these animals. The occurrence of alpha2u-globulin was confirmed by immunohistochemical examination. The accumulation of this protein appears to be a unique feature of male rats and is not known to occur in other species, including man. No signs of neurotoxicity were observed during functional observational

battery as well as measurement of motor activity performed towards the end of the administration period.
Thus, the no-observed-effect-level (NOEL) under the conditions of the present study was 100 ppm for both sexes (about 7 and 8 mg/kg bw/day for males and females) based on adaptive liver effects in both sexes and minor urine findings in males at 1000 ppm which correspond to a dosage of 72 and 83 mg/kg bw/day for males and females (no-observed-adverse-effect-level, NOAEL). The lowest-observed-adverse-effect-level (LOAEL) was found at 10 000 ppm (720 and 801 mg/kg bw/day for males and females) due to liver, kidney and thyroid findings in both sexes. beta-Ionone gave no indication of a mutagenic effect in bacteria or a clastogenic potential in an in vivo mouse micronucleus test. Therefore, there is no indication of a genotoxic potential in vivo. No studies that would be considered adequate for the evaluation of carcinogenic potential were available. A short-term screening experiment investigating a tumor-promoting potential on mouse skin did not indicate such an effect at a low test concentration. In a well-conducted 90 days study in rats according to OECD TG 408 with administration of the test substance in the diet, beta-ionone did not have the potential to damage the reproductive organs at least up to the highest tested concentration of 10,000 ppm (720 and 801 mg/kg bw/day for males and females) beta-Ionone gave no indication of a mutagenic effect in bacteria or a clastogenic potential in an in vivo mouse micronucleus test. Therefore, there is no indication of a genotoxic potential in vivo. No studies that would be considered adequate for the evaluation of carcinogenic potential were available. A short-term screening experiment investigating a tumor-promoting potential on mouse skin did not indicate such an effect at a low test concentration. In a well-conducted 90 days study in rats according to OECD TG 408 with administration of the test substance in the diet, beta-ionone did not have the potential to damage the reproductive organs at least up to the highest tested concentration of 10,000 ppm (720 and 801 mg/kg bw/day for males and females).
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Section 12 - ECOLOGICAL INFORMATION

Refer to data for ingredients, which follows:
ALPHA-DAMASCONE:

Marine Pollutant:	Yes

■ Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
■ 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.
■ Substances containing unsaturated carbons are ubiquitous in indoor environments. They result from many sources (see below). Most are reactive with environmental ozone and many produce stable products which are thought to adversely affect human health.The potential for surfaces in an enclosed space to facilitate reactions should be considered.

Source of unsaturated substances	Unsaturated substances (Reactive Emissions)	Major Stable Products produced following reaction with ozone.
Occupants (exhaled breath, ski oils, personal care products)	Isoprene, nitric oxide, squalene, unsaturated sterols, oleic acid and other unsaturated fatty acids, unsaturated oxidation products	Methacrolein, methyl vinyl ketone, nitrogen dioxide, acetone, 6MHQ, geranyl acetone, 4OPA, formaldehyde, nonanol, decanal, 9-oxo-nonanoic acid, azelaic acid, nonanoic acid.
Soft woods, wood flooring, including cypress, cedar and silver fir boards, houseplants	Isoprene, limonene, alpha-pinene, other terpenes and sesquiterpenes	Formaldehyde, 4-AMC, pinoaldehyde, pinic acid, pinonic acid, formic acid, methacrolein, methyl vinyl ketone, SOAs including ultrafine particles
Carpets and carpet backing	4-Phenylcyclohexene, 4-vinylcyclohexene, styrene, 2-ethylhexyl acrylate, unsaturated fatty acids and esters	Formaldehyde, acetaldehyde, benzaldehyde, hexanal, nonanal, 2-nonenal
Linoleum and paints/polishes containing linseed oil	Linoleic acid, linolenic acid	Propanal, hexanal, nonanal, 2-heptenal, 2-nonenal, 2-decenal, 1-pentene-3-one, propionic acid, n-butyric acid
Latex paint	Residual monomers	Formaldehyde
Certain cleaning products, polishes, waxes, air fresheners	Limonene, alpha-pinene, terpinolene, alpha-terpineol, linalool, linalyl acetate and other terpenoids, longifolene and other sesquiterpenes	Formaldehyde, acetaldehyde, glycoaldehyde, formic acid, acetic acid, hydrogen and organic peroxides, acetone, benzaldehyde, 4-hydroxy-4-methyl-5-hexen-1-al, 5-ethenyl-dihydro-5-methyl-2(3H)-furanone, 4-AMC, SOAs including ultrafine particles
Natural rubber adhesive	Isoprene, terpenes	Formaldehyde, methacrolein, methyl vinyl ketone
Photocopier toner, printed paper, styrene polymers	Styrene	Formaldehyde, benzaldehyde
Environmental tobacco smoke	Styrene, acrolein, nicotine	Formaldehyde, benzaldehyde, hexanal, glyoxal, N-methylformamide, nicotinaldehyde, cotinine
Soiled clothing, fabrics, bedding	Squalene, unsaturated sterols, oleic acid and other saturated fatty acids	Acetone, geranyl acetone, 6MHO, 40PA, formaldehyde, nonanal, decanal, 9-oxo-nonanoic acid, azelaic acid, nonanoic acid

Soiled particle filters	Unsaturated fatty acids from plant waxes, leaf litter, and other vegetative debris; soot; diesel particles	Formaldehyde, nonanal, and other aldehydes; azelaic acid; nonanoic acid; 9-oxo-nonanoic acid and other oxo-acids; compounds with mixed functional groups (=O, -OH, and -COOH)
Ventilation ducts and duct liners	Unsaturated fatty acids and esters, unsaturated oils, neoprene	C5 to C10 aldehydes
"Urban grime"	Polycyclic aromatic hydrocarbons	Oxidized polycyclic aromatic hydrocarbons
Perfumes, colognes, essential oils (e.g. lavender, eucalyptus, tea tree)	Limonene, alpha-pinene, linalool, linalyl acetate, terpinene-4-ol, gamma-terpinene	Formaldehyde, 4-AMC, acetone, 4-hydroxy-4-methyl-5-hexen-1-al, 5-ethenyl-dihydro-5-methyl-2(3H) furanone, SOAs including ultrafine particles
Overall home emissions	Limonene, alpha-pinene, styrene	Formaldehyde, 4-AMC, pinonaldehyde, acetone, pinic acid, pinonic acid, formic acid, benzaldehyde, SOAs including ultrafine particles

Abbreviations: 4-AMC, 4-acetyl-1-methylcyclohexene; 6MHQ, 6-methyl-5-heptene-2-one, 4OPA, 4-oxopentanal, SOA, Secondary Organic Aerosols

Reference: Charles J Weschler; Environmental Helath Perspectives, Vol 114, October 2006.

- For alkenes (olefins)

Environmental fate:

The potential for exposure of aquatic organisms to members of the higher olefins will be influenced by their physico-chemical properties. The predicted or measured water solubilities of these olefins range from 50 mg/L at 20 C for hexene to 0.00015 mg/L at 25 C for 1-octadecene, and to 6.33 [E-23] mg/L at 25 C for C54 alpha olefin, which suggests there is a lower potential for the larger olefins to be bioavailable to aquatic organisms due to their low solubilities. Their vapor pressures range from 230.6 hPa at 25 C for hexene to 0.00009 hPa at 25 C for 1-octadecene, and to 1.13 [E-16] hPa at 25 C for C54 alpha olefin, which suggests the shorter chain olefins will tend to partition to the air at a significant rate and not remain in the other environmental compartments for long periods of time; while the longer chain olefins will tend to partition primarily to water, soil or sediment, depending on water solubility and sorption behavior. The predicted soil adsorption coefficients (Koc) range from 149 for C6 to 230,800 for C18 and to 1.0 [E10] for C54, indicating increasing partitioning to soil/sediment with increasing carbon number. Level I fugacity modelling predicts that the C6-13 olefins would partition primarily to air, while the C16 and longer chain olefins would partition primarily to soil. Results of Level III fugacity modelling suggest that the C6 -8 olefins will partition primarily to the water compartment; and, as the chain length increases beyond C10, soil and sediment become the primary compartments. These chemicals have a very low potential to hydrolyse and do not photodegrade directly. However, in the air, all members of the category are subject to atmospheric oxidation from hydroxyl radical attack, with calculated degradation half- lives of 1.8 to 4.8 hours. C6 -30 olefins have been shown to degrade to an extent of approximately 8-92% in standard 28 day biodegradation tests. These results were not clearly correlated with carbon number or any other identifiable parameter; however, the weight of evidence shows that the members of the higher olefins have potential for degradation in the environment. Volatilisation from water is predicted to occur rapidly (hours to days), with Henry’s Law Constants (bond method) ranging from 0.423 (C6) to 10.7 (C18), and to 2.89 [E5] (C54) atm-m3/mol. Consideration of these degradation processes supports the assessment that these substances will degrade relatively rapidly in the environment and not persist. Based on calculated bioconcentration factors, the C6, C7, and C16 and longer chain length category members are not expected to bioaccumulate (BCF: C6 = 44-46, C7 = 236, C16 = 71-92 and >= C18 = 3.2-4.6). Although the C8 - 15 olefins have BCFs ranging from 313 to 2030, and Kow values ranging from 4.13 to 7.49, and thus are considered to have the potential for bioaccumulation, their physico-chemical properties and fate indicate that there would be limited environmental exposure because of volatility, biodegradability and limited solubility.

Ecotoxicity:

Data indicate that acute aquatic toxicity can be observed for C6 through the C10 olefins (C6: EC/LC50 range of 1-10 mg/L; C7-C10: EC/LC50 range of 0.1-1.0 mg/L), and that toxicity increases with increasing carbon number within that range, which is consistent with increasing Kow values (3.07 -5.12). Above a chain length of 10, toxicity is not observed within the limits of solubility. However, data indicate that chronic aquatic toxicity can be observed in the C10 olefins (EC10 = 20.0 ug/L, EC50= 28.1 ug/L, NOEC = 19.04 ug/L). Data also suggest that aquatic toxicity does not differ with bond location or presence of branching.

- Ionones, damascones and other structurally related materials are ubiquitous in the environment.

Environmental fate:

For beta-ionone: beta-Ionone possesses properties indicating a hazard for the environment.

The colorless to yellowish liquid beta-ionone has a water solubility of about 0.169 g/l and a vapor pressure of about 0.009 hPa at 25 C. The measured log Kow of 4.0 at 25 C, the calculated log Koc of 2.80 - 3.34 and the calculated BCF of 501 indicate a potential for bio- and geoaccumulation. According to distribution modeling using Mackay Level I, water (34 %), soil (27 %), sediment (27 %) and air (12 %) are the main targets for the compound. beta-Ionone is with > 70 % (within 28 days, 10-day-window criteria fulfilled) readily biodegradable according to OECD criteria. In the atmosphere, it will be rapidly photodegraded by reactions with OH radicals (calculated t1/2: 1.6 hours) and ozone (calculated t1/2: 18 minutes).

Ecotoxicity:

Results on acute aquatic toxicity are available for fish (Pimephales promelas; LC50 (96 hours): 5.1 mg/l), invertebrates (Daphnia magna; EC50 (48 hours): 3.7 mg/l) and algae (Scenedesmus subspicatus; EuC50 (72 hours): 22.2 mg/l; EbC50 (72 hours): 21.2 mg/l). Based on these acute toxicity studies, beta-ionone is considered as toxic to aquatic organisms. No results on prolonged or chronic toxicity to aquatic organisms are available. According to the EU risk assessment procedure, a PNECaqua of 3.7 ug/l was obtained by applying an assessment factor of 1000 on the lowest L(E)C50 value, the result of the test with Daphnia magna.

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- DO NOT discharge into sewer or waterways.

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility

alpha-damascone	HIGH	LOW	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 ALPHA-DAMASCONE)

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 alpha-damascone)

Section 15 - REGULATORY INFORMATION

REGULATIONS

alpha-damascone (CAS: 23726-93-4,43052-87-5) is found on the following regulatory lists;
"Canada Non-Domestic Substances List (NDSL)","US Toxic Substances Control Act (TSCA) - Inventory"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

■ Potentially explosive peroxides may form on standing.*.
■ Ingestion may produce health damage*.
■ May produce discomfort of the respiratory system*.
■ Possible respiratory sensitizer*.
■ Vapors potentially cause drowsiness and dizziness*.
* (limited evidence).

Ingredients with multiple CAS Nos

Ingredient Name	CAS
alpha-damascone	23726-93-4, 43052-87-5

■ 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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