

Methyl benzoate

sc-215338



The Power is Question

Material Safety Data Sheet

Hazard Alert Code
Key:

EXTREME

HIGH

MODERATE

LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

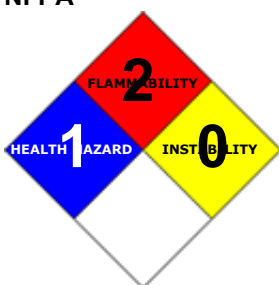
PRODUCT NAME

Methyl benzoate

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

Occurs naturally in oils of clove, ylang ylang and tuberose. Used in perfumery; solvent for cellulose esters and ethers, resins and rubber; flavouring.

SYNONYMS

C8-H8-O2, C6H4CO2CH3, "methyl benzenecarboxylate", "benzoic acid, methyl ester", "Essence of Niobe", "Niobe Oil", "Oil of Niobe", "Oxidate Le", "peau D' Espagne"

Section 2 - HAZARDS IDENTIFICATION

CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

Harmful if swallowed.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

■ Accidental ingestion of the material may be harmful; animal experiments indicate that ingestion of less than 150 gram may be fatal or may produce serious damage 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 .
- Skin contact with the material may damage the health of the individual; systemic effects may result following absorption.
- 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

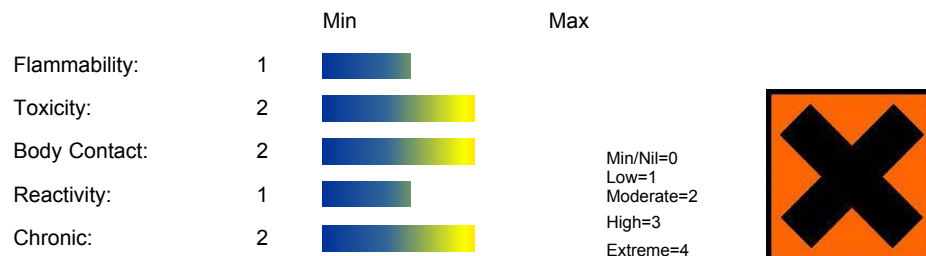
- Inhalation of vapours may cause drowsiness and dizziness. This may be accompanied by narcosis, reduced alertness, loss of reflexes, lack of coordination and vertigo.
- There is some evidence to suggest that the material can cause respiratory irritation in some persons. The body's response to such irritation 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

- Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.
- Chronic solvent inhalation exposures may result in nervous system impairment and liver and blood changes. [PATTYS].

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

HAZARD RATINGS



NAME	CAS RN	%
methyl benzoate	93-58-3	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

- IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY.
- Where Medical attention is not immediately available or where the patient is more than 15 minutes from a hospital or unless instructed otherwise:
 - For advice, contact a Poisons Information Center or a doctor.
 - Urgent hospital treatment is likely to be needed.
 - If conscious, give water to drink.
 - INDUCE vomiting with fingers down the back of the throat, ONLY IF CONSCIOUS. Lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.

NOTE: Wear a protective glove when inducing vomiting by mechanical means.

- In the mean time, qualified first-aid personnel should treat the patient following observation and employing supportive measures as indicated by the patient's condition.
- If the services of a medical officer or medical doctor are readily available, the patient should be placed in his/her care and a copy of the MSDS should be provided. Further action will be the responsibility of the medical specialist.
- If medical attention is not available on the worksite or surroundings send the patient to a hospital together with a copy of the MSDS.

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

- for poisons (where specific treatment regime is absent):

BASIC TREATMENT

- Establish a patent airway with suction where necessary.
- Watch for signs of respiratory insufficiency and assist ventilation as necessary.
- Administer oxygen by non-rebreather mask at 10 to 15 l/min.
- Monitor and treat, where necessary, for pulmonary edema .
- Monitor and treat, where necessary, for shock.
- Anticipate seizures .
- DO NOT use emetics. Where ingestion is suspected rinse mouth and give up to 200 ml water (5 ml/kg recommended) for dilution where patient is able to swallow, has a strong gag reflex and does not drool.

ADVANCED TREATMENT

- Consider orotracheal or nasotracheal intubation for airway control in unconscious patient or where respiratory arrest has occurred.
- Positive-pressure ventilation using a bag-valve mask might be of use.
- Monitor and treat, where necessary, for arrhythmias.
- Start an IV D5W TKO. If signs of hypovolemia are present use lactated Ringers solution. Fluid overload might create complications.
- Drug therapy should be considered for pulmonary edema.
- Hypotension with signs of hypovolemia requires the cautious administration of fluids. Fluid overload might create complications.
- Treat seizures with diazepam.
- Proparacaine hydrochloride should be used to assist eye irrigation.

BRONSTEIN, A.C. and CURRANCE, P.L.

EMERGENCY CARE FOR HAZARDOUS MATERIALS EXPOSURE: 2nd Ed. 1994.

Treat symptomatically.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Not available
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	1.094
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.

May emit poisonous fumes.

May emit corrosive fumes.

FIRE INCOMPATIBILITY

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

PERSONAL PROTECTION

Glasses:

Safety Glasses.

Chemical goggles.

Gloves:

Respirator:

Type A Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

-
- Remove all ignition sources.
- 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

- 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.

ACUTE EXPOSURE GUIDELINE LEVELS (AEGLE) (in ppm)

AEGLE 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.

AEGLE 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.

AEGLE 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

-
- 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.

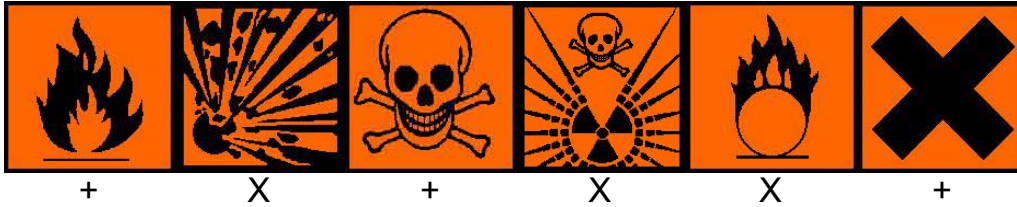
RECOMMENDED STORAGE METHODS

-
- 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.
- No smoking, naked lights or ignition sources.
- 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 preventions

+: May be stored together

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

The following materials had no OELs on our records

- methyl benzoate: CAS:93-58-3

MATERIAL DATA

METHYL BENZOATE:

■ 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.

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

■ General exhaust is adequate under normal operating conditions. Local exhaust ventilation may be required in special circumstances. If risk of overexposure exists, wear an approved respirator. An approved respirator (supplied air type) may be required in special circumstances. Correct fit is essential to ensure adequate protection. Provide adequate ventilation in warehouses and enclosed storage areas.

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.

Sinks in water.

State	Liquid	Molecular Weight	136.15
Melting Range (°F)	10.4	Viscosity	Not Available
Boiling Range (°F)	388.4- 390.2	Solubility in water (g/L)	Immiscible
Flash Point (°F)	181.004	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)	1.094
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	4.69
Volatile Component (%vol)	Not available	Evaporation Rate	Not available

APPEARANCE

Clear, colourless, oily liquid with fragrant odour; does not mix with water. Soluble in alcohol, ether, methanol and fixed oils.

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

methyl benzoate

TOXICITY AND IRRITATION

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

TOXICITY	IRRITATION
Oral (rat) LD50: 2100 mg/kg	Skin (rabbit):10mg/24h(open)-Mild
Oral (rabbit) LD50: 1177 mg/kg	Eye (rabbit): 500 mg/24h - Mild
Oral (mouse) LD50: 3330 mg/kg	Eye (rabbit): 500 mg (open)
Oral (rabbit) LD50: 2170 mg/kg	

Oral (guinea pig) LD50: 4100 mg/kg

- The material may be irritating to the eye, with prolonged contact causing inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis.

The material may cause skin irritation after prolonged or repeated exposure and may produce on contact skin redness, swelling, the production of vesicles, scaling and thickening of the skin.

For certain benzyl derivatives:

All members of this group (benzyl, benzoate and 2-hydroxybenzoate (salicylate) esters) contain a benzene ring bonded directly to an oxygenated functional group (aldehyde or ester) that is hydrolysed and/or oxidised to a benzoic acid derivative. As a stable animal metabolite, benzoic acid derivatives are efficiently excreted primarily in the urine. These reaction pathways have been reported in both aquatic and terrestrial species. The similarity of their toxicologic properties is a reflection their participation in these common metabolic pathways.

In general, members of this group are rapidly absorbed through the gastrointestinal tract, metabolised primarily in the liver, and excreted in the urine either unchanged or as conjugates of benzoic acid derivatives. At high doses, conjugation pathways (e.g., glycine) may be saturated; in which case, free benzoic acid is excreted unchanged. Absorption, distribution and excretion studies have been conducted several members of this group and structural relatives. These substances exhibit remarkably similar patterns of pharmacokinetics and metabolism. The benzyl, benzoate, and 2-hydroxybenzoate (salicylate) esters which comprise this category are hydrolysed to the corresponding alcohols and carboxylic acids. The benzyl alcohol and benzaldehyde derivatives are oxidised to the corresponding benzoic acid derivatives that are subsequently excreted unchanged or as glycine or glucuronic acid conjugates. If methoxy or phenolic functional groups are present on the benzene ring, additional minor metabolic options become available. O-demethylation yields the corresponding phenol that is subsequently excreted as the glucuronic acid or sulfate conjugates. At high dose levels, gut microflora may act to produce minor amounts of reduction metabolites.

Acute toxicity: Oral LD50 values ranged from 887 to greater than 5,000 mg/kg bw demonstrating the low to moderate toxicity of these compounds.

Repeat dose toxicity: Overall, numerous repeat-dose studies using various routes of exposure have been conducted in different animal species with members of this chemical category or their close structural relatives. It is important to note that all the benzyl derivatives in this category are eventually metabolised to a common metabolite, benzoic acid, and are rapidly excreted in the urine as benzoic acid or as its glycine, sulfate, or glucuronic acid conjugate. For this reason, the repeat-dose studies currently available provide adequate support for the safety of the benzyl derivatives. Moreover, the levels at which no adverse effects were reported were sufficiently high to accommodate any potential differences among the members of the category.

Reproductive toxicity: Several reproductive toxicity studies have been conducted with representatives of this group and produced no evidence of reproductive toxicity. As with the repeat-dose studies, the benzyl derivatives generally follow the similar metabolic pathways and the studies conducted provide an adequate database for this endpoint. In addition, the dose levels tested provide margins of safety large enough to accommodate any differences among the group.

Developmental toxicity: Representative substances from this group were tested for developmental toxicity with uniform results, and indicated no teratogenic potential in the absence of maternal toxicity. Again, the representative substances undergo similar metabolism to the entire benzyl derivative group and therefore, provide an adequate representation for this endpoint.

Genetic toxicity: Overall, in vitro and in vivo genotoxicity studies have been conducted with substances representing the structural characteristics of the benzyl category. The results of these studies were predominantly negative demonstrating a low order of genotoxic potential. Limited positive and/or equivocal findings have been reported for 3 aldehydes and benzyl acetate, but, in most cases, other studies of the same endpoint with same test substance show no activity. Most importantly, in vivo studies on benzaldehyde derivatives and closely related benzyl esters have all yielded negative results. These negative in vivo genotoxicity assays are supported by the lack of tumorigenicity in chronic animal studies with representatives of this group.

Data available for more than 100 in vitro genotoxicity assays for 9 members of the category and five metabolic precursors or metabolites of benzyl derivatives indicate a low genotoxic potential for members of this chemical category. Equivocal results have been reported mainly for aromatic aldehydes in the MLA and ABS assays.

Section 12 - ECOLOGICAL INFORMATION

Refer to data for ingredients, which follows:

METHYL BENZOATE:

■ log Pow (Verschueren 1983): 2.12

■ For certain benzyl derivatives:

Environmental fate:

All members of this group (benzyl, benzoate and 2-hydroxybenzoate (salicylate) esters) contain a benzene ring bonded directly to an oxygenated functional group (aldehyde or ester) that is hydrolysed and/or oxidised to a benzoic acid derivative:

Photodegradation: The calculated half lives for hydroxyl radical reactions range from 4.7 to 64.5 hours. The calculated photodegradation half-lives for three benzaldehyde derivatives in this chemical category are in the narrow range from 4.7 hours for m-methoxy-p-hydroxybenzaldehyde to 7.2 hours for the less substituted derivative benzaldehyde. The relative half-lives reflect the increased reactivity of a phenolic OH group. The half-lives for the aldehydes are shorter than those for the corresponding benzyl and benzoate esters in this category (12.7 for methyl benzoate to 64.5 hours for methyl p-methylbenzoate). Generally, the carboxylate function of the ester is more stable to reaction with hydroxyl radicals than the aldehyde function. The calculated half lives for hydroxyl radical reactions range from 4.7 to 64.5 hours. The calculated photodegradation half-lives for three benzaldehyde derivatives in this chemical category are in the narrow range from 4.7 hours for m-methoxy-p-hydroxybenzaldehyde to 7.2 hours for the less substituted derivative benzaldehyde. The relative half-lives reflect the increased reactivity of a phenolic OH group. The half-lives for the aldehydes are shorter than those for the corresponding benzyl and benzoate esters in this category (12.7 for methyl benzoate to 64.5 hours for methyl p-methylbenzoate). Generally, the carboxylate function of the ester is more stable to reaction with hydroxyl radicals than is the aldehyde function. The presence of an aromatic phenol function capable of undergoing ready hydrogen abstraction of the phenolic hydroxyl group decreases predicted photodegradation half-lives. Therefore, the methyl, pentyl and benzyl esters of 2-hydroxybenzoic acid have calculated half-lives of 11.6, 7.6, and 7.4 hours, respectively

Stability in Water: Benzaldehydes in this group cannot hydrolyse. However, they are likely to be slowly oxidized to their corresponding acids. The calculated hydrolysis half-lives for esters range from 20 days at pH 8 and 198 days at pH 7 for benzyl acetate to 1.1 years at pH 8 and 10.8 years at pH 7 for methyl p-methylbenzoate. Benzyl acetate, like several other benzyl esters, was shown to be 50% hydrolysed in 2 hours at pH 7.5 in the presence of pancreatin in an in vitro simulation experiment. These esters are all expected to be readily hydrolysed in vivo.

Biodegradation: All are readily and ultimately biodegradable using a standard OECD 301B test or 301F protocol. The parent acid benzoic acid, its sodium salt, and 2-hydroxybenzoic acid were all readily biodegradable in a COD (chemical oxygen demand) test. Since hydrolysis of the esters and ready oxidation of the aldehydes yields corresponding acid derivatives, the data on benzoic acid, its sodium salt, and 2-hydroxybenzoic acid validate the observations that the aldehydes and esters in this chemical category are readily biodegradable.

Ecotoxicity:

Experimental data indicate a low to moderate toxicity for the benzyl derivatives. Benzyl esters and 2-hydroxybenzoate esters (salicylates) exhibit higher acute toxicity to fish than do benzoate esters or benzaldehyde derivatives. Measured values for benzyl and salicylate esters are in the 1-5 mg/l range with salicylates being slightly more toxic. Benzoate ester and benzaldehyde derivatives exhibit 96-hour LC50 values above 10 mg/L

Benzaldehyde derivatives exhibit lower acute toxicity compared to the parent substance.

Fish LC50 (14-d): guppy 0.17 mg/l (benzaldehyde)

Fish LC50 (96 h): guppy 88-116 mg/l (m-methoxy-p-hydroxybenzaldehyde)

Fish LC50 (96 h): 13-23.5 mg/l (benzaldehyde, p-methoxybenzaldehyde, m-methoxy-p-hydroxybenzaldehyde; estimated values).

Acute toxicity for aquatic invertebrates parallels that for fish in the benzyl chemical category. Benzoate esters exhibit moderate experimental and calculated acute toxicity to invertebrates.

■ DO NOT discharge into sewer or waterways.

log Kow: 2.12

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
methyl benzoate	LOW		LOW	HIGH

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

NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: DOT, IATA, IMDG

Section 15 - REGULATORY INFORMATION

methyl benzoate (CAS: 93-58-3) is found on the following regulatory lists;

"IMO MARPOL 73/78 (Annex II) - List of Noxious Liquid Substances Carried in Bulk", "OECD Representative List of High Production Volume (HPV) Chemicals", "US - New Jersey Right to Know Hazardous Substances", "US DOE Temporary Emergency Exposure Limits (TEELs)", "US EPA High Production Volume Program Chemical List", "US Food Additive Database", "US Toxic Substances Control Act (TSCA) - Inventory"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

- Skin contact may produce health damage*.
- Cumulative effects may result following exposure*.
- May produce discomfort of the respiratory system*.
- Vapors potentially cause drowsiness and dizziness*.

* (limited evidence).

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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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Issue Date: Nov-16-2008

Print Date: Apr-21-2010