Vanillin

sc-251423

Material Safety Data Sheet

Hazard Alert Code Key:	EXTREME	HIGH	MODERATE	LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME
Vanillin

STATEMENT OF HAZARDOUS NATURE
CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA


SUPPLIER
Santa Cruz Biotechnology, Inc.
2145 Delaware Avenue
Santa Cruz, California 95060
800.457.3801 or 831.457.3800

EMERGENCY
ChemWatch
Within the US & Canada: 877-715-9305
Outside the US & Canada: +800 2436 2255
(1-800-CHEMCALL) or call +613 9573 3112

SYNONYMS
C8-H8-O3, 4-(HO)C6H3-3-(OCH3)CHO, 4-hydroxy-3-methoxybenzaldehyde, 4-hydroxy-m-anisaldehyde, p-hydroxy-m-methoxybenzaldehyde, 3-methoxy-4hydroxy-benzaldehyde, methyl-protocatechualdehyde, vanilla, "vanillic aldehyde", p-vanillin, Lioxin, Zimco

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	2		
Body Contact:	0		
Reactivity:	1		
Chronic:	2		

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

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 material is not thought to be an irritant, direct contact with the eye may cause transient discomfort characterized by tearing or conjunctival redness (as with windburn).
Slight abrasive damage may also result.

SKIN

■ Skin contact is not thought to produce harmful health effects (as classified using animal models).
Systemic harm, however, has been identified following exposure of animals by at least one other route and 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 is not thought to produce either adverse health effects or irritation of the respiratory tract following inhalation (as classified using animal models).
Nevertheless, adverse effects have been produced following exposure of animals by at least one other route and good hygiene practice requires that exposure be kept to a minimum and that suitable control measures be used in an occupational setting.
■ Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled.

CHRONIC HEALTH EFFECTS

■ Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.
Long term exposure to high dust concentrations may cause changes in lung function i.e. pneumoconiosis; caused by particles less than 0.5 micron penetrating and remaining in the lung.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
vanillin	121-33-5	>99

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:

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.

SKIN

■ If skin or hair contact occurs: · Flush skin and hair with running water (and soap if available). · Seek medical attention in event of irritation.

INHALED

· If dust is inhaled, remove from contaminated area. · Encourage patient to blow nose to ensure clear passage of breathing. · If irritation or discomfort persists seek medical attention.

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.
Treat symptomatically.

Section 5 - FIRE FIGHTING MEASURES

Vapor Pressure (mmHg):	0.975 @ 107 C
Upper Explosive Limit (%):	Not available.
Specific Gravity (water=1):	1.056

Lower Explosive Limit (%):	Not available.

EXTINGUISHING MEDIA
· Foam.
· Dry chemical powder.

FIRE FIGHTING
· Alert Emergency Responders and tell them location and nature of hazard.
· Wear breathing apparatus plus protective gloves.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS
· Combustible solid which burns but propagates flame with difficulty.
· Avoid generating dust, particularly clouds of dust in a confined or unventilated space as dusts may form an explosive mixture with air, and any source of ignition, i.e. flame or spark, will cause fire or explosion. Dust clouds generated by the fine grinding of the solid are a particular hazard; accumulations of fine dust may burn rapidly and fiercely if ignited.
Combustion products include: carbon monoxide (CO), carbon dioxide (CO_2), other pyrolysis products typical of burning organic material.
May emit poisonous 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:
Chemical goggles.
Gloves:
Respirator:
Particulate

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS
· Remove all ignition sources.
· Clean up all spills immediately.
· Avoid contact with skin and eyes.
· Control personal contact by using protective equipment.
· Use dry clean up procedures and avoid generating dust.
· Place in a suitable, labelled container for waste disposal.
MAJOR SPILLS
■ Moderate hazard.
· CAUTION: Advise personnel in area.
· Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING
· Avoid all personal contact, including inhalation.
· Wear protective clothing when risk of exposure occurs.
Empty containers may contain residual dust which has the potential to accumulate following settling. Such dusts may explode in the presence of an appropriate ignition source.
· Do NOT cut, drill, grind or weld such containers.
· In addition ensure such activity is not performed near full, partially empty or empty containers without appropriate workplace safety authorisation or permit.

RECOMMENDED STORAGE METHODS
■ Glass container.
· Polyethylene or polypropylene container.
· Check all containers are clearly labelled and free from leaks.

STORAGE REQUIREMENTS
· Store in original containers.
· Keep containers securely sealed.
Air and moisture sensitive

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m^3	STEL ppm	STEL mg/m^3	Peak ppm	Peak mg/m^3	TWA F/CC	Notes
US AIHA Workplace Environmental	vanillin (Vanillin)		10						

Exposure Levels (WEELs)				
US - California Permissible Exposure Limits for Chemical Contaminants	vanillin (Particulates not otherwise regulated Respirable fraction)	5		(n)
US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants	vanillin (Particulates not otherwise regulated Respirable fraction)	5		
US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants	vanillin (Particulates not otherwise regulated (PNOR)(f)-Respirable fraction)	5		
US - Michigan Exposure Limits for Air Contaminants	vanillin (Particulates not otherwise regulated, Respirable dust)	5		
Canada - Prince Edward Island Occupational Exposure Limits	vanillin (Particles (Insoluble or Poorly Soluble) [NOS] Inhalable particles)	10		See Appendix B current TLV/BEI Book

ENDOELTABLE

PERSONAL PROTECTION



RESPIRATOR

Particulate

Consult your EHS staff for recommendations

EYE

· Safety glasses with side shields

· Chemical goggles.

HANDS/FEET

■ 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.

Experience indicates that the following polymers are suitable as glove materials for protection against undissolved, dry solids, where abrasive particles are not present.

· polychloroprene

· nitrile rubber

· butyl rubber

· fluorocaoutchouc

· polyvinyl chloride

Gloves should be examined for wear and/ or degradation constantly.

OTHER

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

ENGINEERING CONTROLS

· Local exhaust ventilation is required where solids are handled as powders or crystals; even when particulates are relatively large, a certain proportion will be powdered by mutual friction.
· Exhaust ventilation should be designed to prevent accumulation and recirculation of particulates in the workplace.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Solid.
Does not mix with water.
Sinks in water.

State	Divided solid	Molecular Weight	152.16
Melting Range (°F)	176- 179.6	Viscosity	Not Available
Boiling Range (°F)	338 @ 20 hPa	Solubility in water (g/L)	Partly miscible
Flash Point (°F)	Not available	pH (1% solution)	<7
Decomposition Temp (°F)	Not available.	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available.	Vapor Pressure (mmHg)	0.975 @ 107 C
Upper Explosive Limit (%)	Not available.	Specific Gravity (water=1)	1.056
Lower Explosive Limit (%)	Not available.	Relative Vapor Density (air=1)	5.3
Volatile Component (%vol)	Negligible	Evaporation Rate	Not applicable

APPEARANCE

White to very slightly yellow needle crystals, slightly soluble in water. Pleasant vanilla odour and taste. Freely soluble in alcohol chloroform, ether, carbon disulphide, glacial acetic acid, oils and solutions of alkali hydroxides. Affected by light. Slowly oxidises on exposure to moist air. Solutions are weakly acid to litmus. A natural or synthetic product.

log Kow 1.26

Material	Value

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

· Presence of incompatible materials.
· Product is considered stable.

STORAGE INCOMPATIBILITY

■ Avoid reaction with oxidizing agents, bases and strong reducing agents.

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

Section 11 - TOXICOLOGICAL INFORMATION

VANILLIN

TOXICITY AND IRRITATION

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

TOXICITY	IRRITATION
Oral (rat) LD50: 1580 mg/kg	Nil Reported
Intraperitoneal (rat) LD50: 1160 mg/kg	
Intraperitoneal (mouse) LD50: 475 mg/kg	
Oral (guinea pig) LD50: 1400 mg/kg	
Subcutaneous (Rat) LD50: 1500 mg/kg	
Intravenous (Dog) LD: 1320 mg/kg	
Oral (Mouse) LD50: 1480 mg/kg	

■ 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.

For vanillin:

Metabolism studies in rats have shown that vanillin is metabolised to a number of urinary products, primarily vanillic acid, in both free and conjugated forms. Only minor amounts of unmetabolised vanillin is excreted. One person who ingested 100 mg vanillin excreted 96 mg as vanillic acid (94% of the dose) in the next 24 hour period.

Dermal studies. Vanillin was tested in the closed patch test on healthy normals and on subjects with dermatoses. Both in the healthy persons and in those with dermatoses vanillin was negative in all tests. No sign of irritation or erythema was observed.

A patch test was carried out on 30 workers in a vanillin factory and compared with 15 controls. About half of the workers had dermatitis. Vanillin was applied undiluted and removed after 48 hours. No signs of irritation or sensitisation was observed with vanillin.

In two different studies, positive reactions to vanillin have been reported in patients who already were sensitised to Balsam of Peru. From these studies vanillin was considered to be a secondary allergen

Repeat dose toxicity: The repeated oral administration studies in rat suggest that the NOEL can be as high as 50,000 ppm (2500 mg/kg/day).

Reproductive toxicity: Most of the repeated dose toxicity studies conducted in different animal species have, however, included both macroscopic and microscopic histopathological evaluation of the reproductive organs with no reported effect of the test substance. Also, throughout the many years of wide use of vanillin, there are no indications that vanillin is toxic to the reproductive system.

Developmental toxicity: In a mouse spot test designed to measure the antimutagenic effect of vanillin, pregnant mice were given 3 successive oral administrations of vanillin at 125-500 mg/kg at 0, 4 and 24 hours after the injection of the mutagen ethylnitrosourea. Vanillin was also given to females in the control group (not given the mutagen). Vanillin was shown to have an antimutagenic effect. Even if this study was designed for another purpose, it indicates that administration of vanillin has no toxic effect on the mouse embryos

Teratogenicity: Vanillin turned out to be non-teratogenic when tested in the developing chicken embryo test. Four exposure conditions were used; injection via the air cell and via the yolk and at two different time points
(0 and 96 hr).

Genetic toxicity: Testing of the potential genotoxicity of vanillin has been conducted in a whole range of tests in bacteria (in vitro), in mammalian cells (in vitro) and in different in vivo test. Testing of potential mutagenicity for vanillin in Ames test, DNA repair test and reverse mutation assays with E. coli are all negative both in the presence and the absence of a metabolic activation system (S9). Few signs of cytogenicity have been observed, even with doses up to 10 mg/plate.

Testing of vanillin mutagenicity in mammalian cells in vitro have shown positive effects in some test systems. Increased number of aberrations has been seen at high vanillin concentrations in human lymphocytes only when gaps are included. The biological significance of gaps are, however, debated and is not alone any proof of genotoxicity. In mouse fibroblasts, vanillin has been shown to induce multinuclear mutations. In two independent studies in human lymphocytes, vanillin induced sister chromatid exchange. High concentrations of vanillin is cytotoxic to mammalian cells. The mutagenicity testing in vitro in mammalian cells indicates a genotoxic potential of vanillin. However, several of these studies were performed at high, unphysiological concentrations that could lead to false positives.

Carcinogenicity: A full 2 years oral feeding carcinogenicity study has been conducted in rats with a negative result. There was no indication of vanillin being an experimental carcinogen. The other tests conducted confirm this finding and some tests even indicate that vanillin reduces the tumourigenicity of carcinogenic treatments. None of the carcinogenicity studies presented have been conducted according to GLP, but

the 2 years study (conducted prior to GLP regulations) seem to hold a high scientific standard and includes an appropriate number of animals and groups
Immunotoxicity: Testing of possible immunotoxicity indicated that vanillin is not immunotoxic, but one study indicated an immunostimulating effect, while another indicated an immunosuppressive effect.
Miosis, somnolence, muscle weakness, coma, respiratory stimulation, maternal effects involving ovaries, fallopian tubes, uterus, cervix and vagina recorded.

Section 12 - ECOLOGICAL INFORMATION

No data

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
vanillin	LOW		LOW	HIGH

GESAMP/EHS COMPOSITE LIST - GESAMP Hazard Profiles

Name / EHS TRN A1a A1b A1 A2 B1 B2 C1 C2 C3 D1 D2 D3 E1 E2 E3 Cas No / RTECS No _____ Alcoholic 293 85 0 0 0 R 0 0 0 0 0 0 1 D 1 beverages / CAS:121- 33- 5 /

Legend: EHS=EHS Number (EHS=GESAMP Working Group on the Evaluation of the Hazards of Harmful Substances Carried by Ships) NRT=Net Register Tonnage, A1a=Bioaccumulation log Pow, A1b=Bioaccumulation BCF, A1=Bioaccumulation, A2=Biodegradation, B1=Acuteaquatic toxicity LC/ECIC50 (mg/l), B2=Chronic aquatic toxicity NOEC (mg/l), C1=Acute mammalian oral toxicity LD50 (mg/kg), C2=Acutemammalian dermal toxicity LD50 (mg/kg), C3=Acute mammalian inhalation toxicity LC50 (mg/kg), D1=Skin irritation & corrosion, D2=Eye irritation& corrosion, D3=Long-term health effects, E1=Tainting, E2=Physical effects on wildlife & benthic habitats, E3=Interference with coastal amenities, For column A2: R=Readily biodegradable, NR=Not readily biodegradable. For column D3: C=Carcinogen, M=Mutagenic, R=Reprotoxic, S=Sensitising, A=Aspiration hazard, T=Target organ systemic toxicity, L=Lunginjury, N=Neurotoxic, I=Immunotoxic. For column E1: NT=Not tainting (tested), T=Tainting test positive. For column E2: Fp=Persistent floater, F=Floater, S=Sinking substances. The numerical scales start from 0 (no hazard), while higher numbers reflect increasing hazard. (GESAMP/EHS Composite List of Hazard Profiles - Hazard evaluation of substances transported by ships)

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. 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.
· Consult manufacturer for recycling options or consult Waste Management Authority for disposal if no suitable treatment or disposal facility can be identified.

Section 14 - TRANSPORTATION INFORMATION

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

Section 15 - REGULATORY INFORMATION

vanillin (CAS: 121-33-5) is found on the following regulatory lists;

"Canada Domestic Substances List (DSL)","International Fragrance Association (IFRA) Survey: Transparency List","OECD Representative List of High Production Volume (HPV) Chemicals","US AIHA Workplace Environmental Exposure Levels (WEELs)","US DOE Temporary Emergency Exposure Limits (TEELs)","US EPA High Production Volume Program Chemical List","US EPA Master Testing List - Index I Chemicals Listed","US Food Additive Database","US Toxic Substances Control Act (TSCA) - Inventory","US TSCA Section 8 (a) - Preliminary Assessment Information Rules (PAIR) - Reporting List","US TSCA Section 8 (d) - Health and Safety Data Reporting"

Section 16 - OTHER INFORMATION

ND
Substance CAS Suggested codes vanillin 121- 33- 5

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■ Classification of the preparation 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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