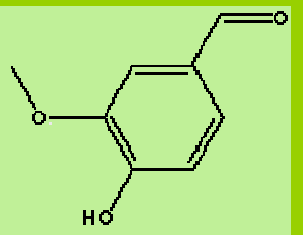
VANILLIN



PRODUCT IDENTIFICATION	
CAS NO.	121-33-5; 52447-63-9; 8014-42-4
EINECS NO.	204-465-2
FORMULA	$HOC_6H_3(OCH_3)CHO$
MOL WT.	152.15
H.S. CODE	2912.41.0000
TOXICITY	Oral rat LD50: 1580 mg/kg
SYNONYMS	4-Hydroxy-3-methoxybenzaldehyde; 3-Methoxy-4-hydroxybenzaldehyde; p-Hydroxy-m-methoxybenzaldehyde; Vanillic aldehyde; 2-Methoxy-4-formylphenol; 4-Formyl-2-methoxyphenol; 4-Hydroxy-5-methoxybenzaldehyde; Vanilla; 4-Hydroxy-m-anisaldehyde; Methyl protocatechualdehyde; p-Vanillin; 4-Hydroxy-m-anisaldehyde; Vanillaldehyde; m-Methoxy-p-hydroxybenzaldehyde; Protocatechualdehyde 3-methyl ether; 2-Methoxy-4-formylphenol;
SMILES	c1(cc(ccc1O)C=O)OC
CLASSIFICATION	Aldehyde, Phenol ether, Anticonvulsant, Antimutagenic, Antioxidant, Pharmaceutic aid, Flavors and Fragrances agent, Perfume ingredient

PHYSICAL AND CHEMICAL PROPERTIES	
PHYSICAL STATE	White to light yellow powder or crystals
MELTING POINT	81 - 83 C
BOILING POINT	285 C
SPECIFIC GRAVITY	1.056
SOLUBILITY IN WATER	Slightly soluble (1.10E+04 mg/l at 25 C)
SOLUBILITY IN SOLVENTS	Freely soluble in glacial acetic acid, alcohol, chloroform, ether, carbon disulfide and methanol. Soluble in aq. solutions of alkali hydroxides
VAPOR DENSITY	5.2
NFPA RATINGS	Health: 1; Flammability: 1; Reactivity: 0
pKa	7.396 (Dissociation Constant at 20 C)
log Pow	1.21 (Octanol-water)
VAPOR PRESSURE	(mmHg at 25 C)
HENRY'S LAW	2.15E-09 (atm-m3/mole at 25 C)
OH RATE	2.73E-11 (cm3/molecule-sec at 25 C Atmospheric)
REFRACTIVE INDEX	
AUTOIGNITION	
FLASH POINT	147 C
STABILITY	Slowly oxidizes in contact with moist and air. Light sensitive

GENERAL DESCRIPTION & EXTERNAL LINKS

Vanilla is a plant belongs to the family Orchidaceae, native to tropical American forests. Both V. planifoʗlia Andr. (Mexican or Bourbon vanilla) and V. tahitenʗsis Moor (Tahitian vanilla) have fruits called vanilla beans which are picked before fully matured. Vanilla is a choice of flavoring agnet prepared from vanilla beans with or without the addition of sugar, dextrose, or glycerol. Vanilla extract contains soluble matter from not less than 10 grams of vanilla beans in 100 milliliters. Vanillin (chemically 4-hydroxy-3-methoxybenzaldehyde) is a constituent of vanilla or is prepared synthetically.

Vanillic acid: the oxidation form of vanillin. The chemical designation is 4-hydroxy-3-

methoxybenzoic acid.

Ethamivan: the diethylamide of vanillic acid; used as a central nervous system stimulant, respiratory stimulant, and analeptic.

Ethyl vanillin: white to pale yellow crystal; melting 76.5 C; having 3.5 times stronger flavour and more stable in organic solvents and in storage than vanillin but does not have the true flavour. It is used in pharmaceutical preparations and the food industry as a flavoring agent to replace or strengthen vanilla.

Acetovanillon: white crystal a faint vanilla odor; melting point 115 C; soluble in hot water, alcohol, benzene, chloroform, and ether; used as a cardiotonic drug. Chemical naming is 4'-Hydroxy-3'-methoxyacetophenone.

Is this it the same as Vanilla?:
No. Vanillin is a single molecule, 4-hydroxy-3-methoxybenzaldehyde (much easier to call it Vanillin), whose structure is shown in the image on the right. It's a white crystalline solid, which melts at 81°C. *Vanilla planifola* is an orchid which produces seed pods from which vanilla extracts are obtained; these extracts contain nearly 200 different molecules, of which vanillin is the most important, and most abundant, making up 98% of the eventual vanilla extract. Vanillin itself was first isolated from vanilla pods by Nicholas-Theodore Gobley in 1858 (though he thought that its formula was $C_{10}H_6O_2$, not $C_8H_8O_2$). The biosynthetic pathway starts with phenylalanine.

Synthesis of Vanillin: Vanillin (4-hydroxy-3-methoxybenzaldehyde), a pleasant smelling aromatic compound, occurs naturally in vanilla beans. It is used widely as a flavoring additive for beverages, cooking, and as an aromatic additive for candles, incense, potpourri, fragrances, perfumes, and air fresheners. It may be isolated from the vanilla bean, and is often obtained as a byproduct of the pulp and paper industry by the oxidative breakdown of lignin. It may also be prepared by synthesis. We have developed (equation 1) a convenient two step synthesis of vanillin using electrophilic aromatic substitution, followed by an organometallic methoxylation procedure using copper bromide and sodium methoxide.....

Vanillin was one of seven phenolic compounds studied for their protective properties against hydrogen peroxide-induced DNA damage in human peripheral blood lymphocytes. Vanillin, curcumin, and resveratrol protected against DNA damage induced by 50 ¥ìM H2O2 at a concentration range of 6.25 - 25 ¥ìM....

SALES SPECIFICATION	
APPEARANCE	White to light yellow crystalline powder
PURITY (G.C.)	99.0% min
MELTING POINT	81 - 83 C
LOSS ON DRYING	0.5% max
HEAVY METALS	10ppm max
TRANSPORTATION	
PACKING	
HAZARD CLASS	
UN NO.	
OTHER INFORMATION	
FEMA No. 3107	