**Company: PROCHEM INNOVATIONS** 

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Chemical Formula: C<sub>9</sub>H<sub>8</sub>O<sub>2</sub>

Chemical Name: 3-phenylprop-2-enoic acid

#### Use case:

a. What is the use of this compound?

Cinnamic acid is used in flavourings, synthetic indigo, and certain pharmaceuticals. A major use is as a precursor to produce methyl cinnamate, ethyl cinnamate, and benzyl cinnamate for the perfume industry. It is used for its aroma in perfumes and cosmetics. Cinnamic acid is a precursor to the sweetener aspartame via enzyme-catalysed amination to give phenylalanine. Cinnamic acid can dimerize in non-polar solvents resulting in different linear free energy relationships.

b. Are there any alternatives to this compound? Name a few.

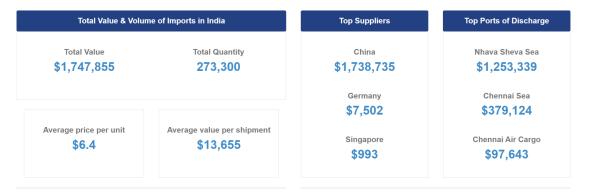
Yes, certainly there are some compounds which can be used as an alternative to this compound. These are

- benzoic acid
- sorbic acid
- c. Why this compound is superior to its alternatives?

Cinnamic acid has demonstrated a broader spectrum of antimicrobial activity compared to sorbic and benzoic acid. It has been found effective against a wider range of microorganisms, including bacteria, fungi, and certain viruses. Cinnamic acid is often perceived to have a milder flavor and odor compared to sorbic and benzoic acid. Cinnamic acid is relatively stable under a wide range of pH conditions, which can make it more versatile for use in formulations with varying pH levels. In contrast, sorbic acid is less stable at lower pH levels, and benzoic acid can undergo degradation in the presence of certain pH-adjusting agents or under high-temperature conditions. Due to these factors we prefer cinnamic acid to be superior than its alternative.

e. Is this compound imported in India? What is the magnitude of imports? Yes, cinnamic acid is imported in India. Average import price for cinnamic acid is \$12.73 i.e. Rs.1057 approximately. The data related to magnitude of import is shown below:

#### Analysis of Import of:



## **Economic feasibility:**

a. What input raw materials are needed for its synthesis (same as reported in the Patent application)?

Benzaldehyde (C<sub>6</sub>H<sub>5</sub>CHO)

Acetic anhydride ((CH<sub>3</sub>CO)<sub>2</sub>O)

Base catalyst (e.g., sodium acetate or pyridine)

Solvent (e.g., toluene or xylene)

b. Provide preliminary economic feasibility based on cost of raw materials, solvents and product selling price.

Price of sodium acetate: Rs. 20/kg

Price of benzaldehyde: Rs. 140/kg

Price of acetic anhydride: Rs. 50/kg

Price of acetic acid: Rs.170/kg

Price of Cinnamic Acid: Rs. 550/kg

Assumption: Assuming 100% yield of cinnamic acid without side reaction.

C<sub>6</sub>H<sub>5</sub>CHO + (CH<sub>3</sub>CO)<sub>2</sub>O + CH<sub>3</sub>COONa → C<sub>0</sub>H<sub>8</sub>O<sub>2</sub> + CH<sub>3</sub>COOH

# Feasibility analysis:

moles of product = (1000\*1000)/148=6756.76

According to reaction stoichiometry, the moles of benzaldehyde and acetic anhydride needed for per mole synthesis of the compound is 1 each.

mass of benzaldehyde: 716.33kg

mass of acetic anhydride: 689.291kg

mass of sodium acetate: 554.136kg

mass of acetic acid formed: 405.46 kg

## **Cost Analysis:**

Cost of benzaldehyde: 140\*716.33 = Rs. 100,286.2

Cost of Acetic Anhydride: 50\*689.291 = Rs. 34,464.55

Cost of Sodium Acetate: 20\*554.136 = Rs. 11,082.72

Total input cost= Rs. 100,286.2+ 34,464.55+ 11,082.72 = Rs. 1,45,833.47

cost of products = Cost of cinnamic acid + Cost of acetic acid

= (550\*1000)+(170\*405.46)

= Rs. 6,18,928.2

Thus Daily profit of production = Rs. 6,18,928.2 - Rs. 1,45,833.47

= Rs. 4,73,094.73

#### References:

uses of Cinnamic acid

import of cinnamic acid

price of sodium acetate

price of toluene solvent

price of acetic anhydride

# List the contributions of each author:

- Author 1 and 2 carried out the market research for chemical trade data.
- Author 3 and 4 prepared the use case.
- Author 1 and 2 looked at economic feasibility and found out the profitability of the production.

| Name             | Roll No | Signature |
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**Applicant:** ProChem Innovations

**CEO:** Nikhil Gupta

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**Chemical Formula:** C<sub>3</sub>H<sub>8</sub>O

Chemical Name: Isopropanol

#### **Use Case:**

a. What is the use of this compound?

Isopropyl alcohol is used, as a solvent for gums, shellac and essential oils, and in quick-drying inks and oils. The compound is a used as a component in body rubs, hand lotions, after-shave lotions, cosmetics and antifreeze products. Isopropanol is used as an intermediate chemical in the manufacturing of glycerol and isopropyl acetate. For medicinal purposes, the compound is used as an antiseptic for skin and instrumentation.

b. Are there any alternatives to this compound? Name a few.

Yes, few compounds can be used as an alternative to isopropanol as depending on the use case. For example: Ethanol, Hydrogen Peroxide and Benzalkonium Chloride can be used as disinfectants. Methanol and Acetone can be used as solvents.

c. Why is this compound superior to its alternatives?

The compound has a rapid rate of evaporation and superior purity characteristics, which make it a safer choice than its alternatives, especially for cleaning sensitive electronic equipment. The compound is considerably less toxic than methanol. Hence, it is a safer choice as a solvent.

d. Is this compound imported in India? What is the magnitude of imports? Yes, this compound is imported in India. The import quota is 132440 metric tonnes for FY24.

#### **Economic Feasibility:**

b. What input raw materials are needed for its synthesis (same as reported in the Patent application)?

The input raw materials needed for the synthesis are:

- a. Acetone
- b. Bimetallic Cu-Al mixed oxide (catalyst)
- c. Hydrogen Stream
- b. Provide preliminary economic feasibility based on cost of raw materials, solvents and product selling price.
  - Cost of raw materials

o Industry grade Acetone: Rs. 39.225/kg

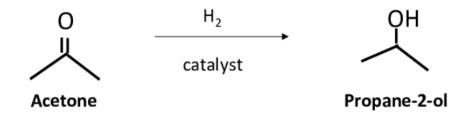
o Hydrogen: Rs 102.75/unit

## Product Selling Price

Isopropanol: Rs 135/kg

## Feasibility Analysis

(The feasibility analysis done below is for 1-mole production of Isopropanol) Reaction:



Assumption: - assuming maximum yield of isopropanol which is 60% (from patent report)

# QUANTITIES OF DIFFERENT MATERIALS: -

For a projected production of 1000 kg/day of Isopropanol: -

Moles of Isopropanol: - (1000\*1000 g)/(60.11 g/mol) = 16636.167 moles

According to reaction stoichiometry, the moles of Acetone and Hydrogen needed for per mole synthesis of the compound is 1 each.

### **COST ANALYSIS:**

Input Cost of Acetone: - Rs (39.225/1000) × 58.08 = Rs 2.28/mole

Input Cost of Hydrogen: - Rs (102.75/1000) × 2 = Rs 0.205/mole

Total Input Cost: - Rs (2.278 + 0.2055) = Rs 2.485/mole

Output Cost of Isopropanol: - Rs (135/1000) × (60.11) = Rs 8.115/mole

Since the %yield is 60%, therefore one mole of isopropanol is produced by 1.67 moles of both of input materials (Acetone and Hydrogen)

Profit for per mole production of Isopropanol is Rs  $(8.115 - 1.67 \times 2.485) = Rs$  3.965/mole

Thus profit for the production of 16636.167 (1000 kg) moles of Isopropanol is:  $3.965 \times 16636.167 = Rs. 65,963.234$ 

Thus, Daily Profit of production: - Rs 65,963.234

#### References:

- a. Isopropyl Alcohol vs Ethanol
- b. General Information about isopropyl alcohol
- c. <u>Isopropyl alcohol imports</u>
- d. Acetone Price
- e. Import analysis and trends of of hydrogen | Zauba
- f. <u>isopropanol Indiamart</u> (Selling price)

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