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Chemical Formula: C₁₂H₁₄O₄

Chemical Name: Diethyl phthalate

Use case:

a. What is the use of this compound?

Diethyl phthalate is currently used through direct addition in cosmetic products and indirectly in fragrances, denaturants, and film formers. The compound finds extensive use in cosmetics (bath preparations, eye shadows, bath soaps, detergents, and nail polish). It is also used as a plasticizer in PVC, a fixative in perfume, a component in insecticide sprays and mosquito repellent.

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

Yes, certain compounds exist that are alternatives for the compound. Example: - Camphor, Di isobutyl Phthalate etc.

c. Why this compound is superior to its alternatives?

The most striking feature of the compound is its biodegradable nature, making it an eco-friendly chemical. The other contemporary chemicals pose a serious threat to the environment. Also, this compound is more effective as a plasticizer and solvent. It is more compatible with a wide variety of materials.

d. Is this compound imported in India? What is the magnitude of imports?

Yes, the compound is imported in India. The import cost is roughly around Rs. 1100 per Unit. Market research forecasts the phthalates market to grow significantly to INR 132,586.98 million by 2030.

Economic feasibility:

a. 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. Phthalic Anhydride
- b. Ethanol
- c. H₂SO₄ conc. (Catalyst)
- d. H20(Solvent)
- e. Caustic Soda
- b. Provide preliminary economic feasibility based on cost of raw materials, solvents and product selling price.
 - Cost of Raw Materials: -
- a. Phthalic Anhydride INR 57/kg
- b. Pure Ethanol INR 34/kg
- c. Conc H2SO4 INR 10/kg
- d. H20 (Solvent) INR 0.0432/kg
- e. Caustic Soda INR 60/kg
 - Product Selling Price: -
- a. Diethyl Phthalate: INR 160/kg
 - **Feasibility Analysis:** (The feasibility analysis done below is for 1-mole production of Diethyl Phthalate)

Reaction: -

$$\begin{array}{c|c} O & H_2SO_4 \text{ (cat)} \\ \hline & EtOH \\ \hline \end{array}$$
 Diethyl phthalate

Assumption: - assuming 100% yield of diethyl phthalate and no side reactions

QUANTITIES OF DIFFERENT MATERIALS: -

For a projected production of 1000 kg/day of Diethyl Phthalate: -

Moles of Diethyl Phthalate: -(1000*1000 g)/(222.24 g/mol) = 4499.64 moles

According to reaction stoichiometry, the moles of Phthalic Anhydride and Ethanol needed for per mole synthesis of the compound is 1 each.

Caustic Soda to be used is 5% of the weight of Diethyl Phthalate being produced.

Since we have 92% (w/w) Ethanol, for 1 mole ethanol (46g) we need 50g of solution which gives the weight of water required: - 50-46 = 4g

The amount of 95% (w/w) Sulphuric acid required is 2 % of Diethyl Phthalate being produced. That is 4.48g of H2So4, that is 4.72 g of the solution is required which means 0.24 g of water as solvent needed.

COST ANALYSIS: -

Input Cost of Phthalic Anhydride: - Rs (57/1000) * 148.5 = Rs 8.46

Input Cost of Ethanol: - Rs (34/1000) *46 = Rs 1.564

However, since the feed requires a 1:2 ratio of Phthalic anhydride and Ethanol thus final input cost of ethanol: is - Rs 1.564*2 = Rs 3.128

Input Cost of water: - Rs (0.0432) * (0.008+0.24) = Rs 0.0107

Input Cost of Sulphuric Acid: - Rs (4.48) * (0.01) = Rs 0.0448

Input Cost of Caustic Soda: - Rs (0.05*222.24) *(0.06) = Rs 0.66672

Total Input Cost: - Rs (8.46 + 3.128 + 0.0107 + 0.0448 + 0.66672) = Rs 12.31

Output Cost of Diethyl Phthalate: - Rs (0.16) * (222.24) = Rs 35.56

Profit for per mole production of Diethyl Phthalate is Rs (35.56 - 12.31) = 23.25

Thus profit for the production of 4499.64 (1000 kg) moles of Diethyl Phthalate Is:- 23.25*4499.64 = Rs. 104616.63

Thus, Daily Profit of production: - 23.25*4499.64 = Rs. 104616.63

References:

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https://dir.indiamart.com/impcat/diethyl-phthalate.html :- Selling price of Diethyl Phthalate

https://dir.indiamart.com/impcat/caustic-soda-flakes.html :- Caustic Soda Price

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extension://efaidnbmnnnibpcajpcglclefindmkaj/https://www.atsdr.cdc.gov/ToxProfiles/tp73-c4.pdf: Information about Product uses, Alternative compounds.

List the contributions of each author:

- Author 1,2 and 3 carried out market research for chemical trade data.
- Author 1 and 3 prepared the use case.
- Author 1 and 2 looked at economic feasibility.

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