

## Nature of Invention: Chemical molecule and synthesis route

**Applicant:** CHEMINOVA

**Inventor:** SHREYA.S. NAIR (211001)

**Chemical Formula:** C<sub>16</sub>H<sub>22</sub>O<sub>4</sub>

**Chemical Name:** Diisobutyl Phthalate

**Chemical synthesis routes:**

### STAGE 1: PREPARATION OF PARA TOLUENE SULFONIC ACID

Raw Materials-

1. Sulfuric Acid
2. Toluene
3. Water(H<sub>2</sub>O)
4. Sodium Hydroxide

Reactants-

- 1.Sulfuric Acid
- 2.Toluene

Step 1:

Toluene+ Sulfuric acid → Para Toluene sulfonic acid + water

Balanced reaction-



- Temperature: 0-10 degree celcius
- Yield: 85-90%
- Time duration: 4-5 hours

Step 2:

Hydrolysis of sulfonic acid esters formed in step 1.

Step 3:

Addition of Sodium Hydroxide or Sodium Carbonate to get pH= 7 to 8.

Step 4:

Purification of PTSA:

By filtration or centrifugation and subsequent recrystallization from water or ethanol.

Final Purity – 99%

## **STAGE 2: Synthesis of DIBP**

### **RAW MATERIALS:**

- Phthalic Anhydride
- Isobutanol
- Para toluene sulfonic acid

### **Reactants:**

- Phthalic Anhydride
- Isobutanol

### **Catalyst:**

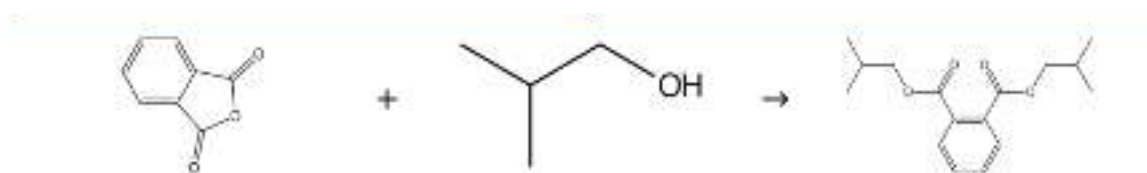
- Para toluene sulfonic acid

### **Step 1:**

## Phthalic Anhydride + Isobutyl Alcohol → DIBP

- Catalyst - Para toluene sulfonic acid

### Balanced reaction-



**Temperature- 300-degree Celsius**

**Yield>90%**

**Time duration- 5-6 hours**

### **Step 2:**

#### **Purification of DIBP-**

Cool the mixture to room temperature and then pour into a separatory funnel. Add water to the separatory funnel and shake vigorously to separate DIBP layer from aqueous layer. Then drain off the aqueous layer and collect DIBP layer in a clean flask and purify by distillation under reduced pressure.

- Final Purity=99.5%
- Time duration- 4 to 8 hours

References – 1. [https://scifinder-n.cas.org/patent-viewer?docuri=bgB1bpD23mjoM9AANTxBsmRpHP8UWkaBeTSLwx\\_gYfM&markedFullTextKey=C-6lwWxYt-](https://scifinder-n.cas.org/patent-viewer?docuri=bgB1bpD23mjoM9AANTxBsmRpHP8UWkaBeTSLwx_gYfM&markedFullTextKey=C-6lwWxYt-)

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