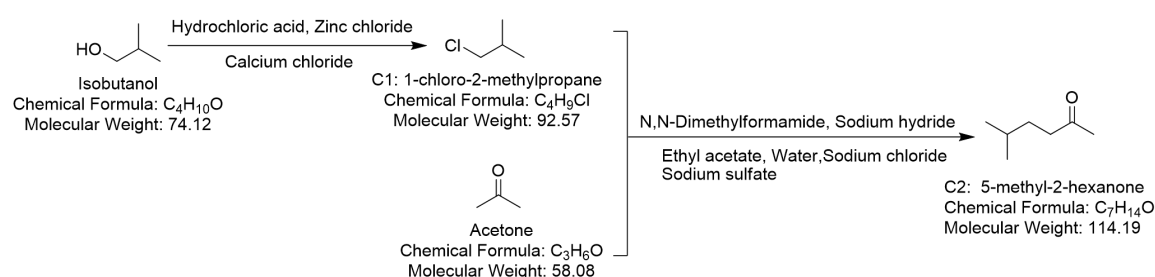




Route of Synthesis

Product: 5-Methyl-2-Hexanone[CAS NO:110-12-3]



Detailed Description of Process

C1 Preparation:

To the mixture of hydrochloric acid(110ml, 35%) and zinc chloride (20.4g, 0.15mol) in a 500ml round bottom flask was added isobutanol(74.1g, 1.0mol) drop-wise with 10 min. The resulting reaction mixture was then reflux with stirring for 2h. The distillates of 1-chloro-2-methylpropane was collected by distillation at 67.5°C-69.0°C and dried by calcium chloride.

C2 Preparation:

To a 500ml flask containing 1-chloro-2-methylpropane(40.0g, 0.43mol) and acetone (60ml, 0.82mol), N, N-dimethylformamide(5.0ml) was charged. The mixture was maintained below 10°C during the slow addition of sodium hydride(22.8g, 0.95mol) over 2h. The solution warmed to 40°C overnight. The reaction was quenched with ice water and extracted with ethyl acetate (300mL) twice. The ethyl acetate extract was washed with brine and dried over sodium sulfate and then evaporated, yielding 5-Methyl-2-hexanone which was yellow liquid.