

PROPARGYL ESTER OF DISUBSTITUTED PHENOXYACETIC ACID

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Abstract: The propargyl ester of disubstituted phenoxyacetic acid is a chemical compound that consists of a phenoxyacetic acid molecule with two substituents attached to the aromatic ring, and an ester group attached to the carboxyl group of the acid. Additionally, the ester group contains a propargyl functional group. The solvents used were ethyl acetate, ethyl alcohol, hexane, acetone, benzene, and toluene. The structure of the synthesized compounds was reliably analyzed using modern IR, ¹H and ¹³C NMR spectroscopy.

Key words: Propargyl ester, phenoxyacetic acid, ethyl acetate, ethyl alcohol, hexane, acetone, benzene, and toluene.

Currently, studies based on triazole derivatives belonging to the class of heterocyclic compounds are very common. This is due to the fact that among five-membered triazole compounds containing three nitrogen atoms, many substances have been found that possessing pharmacological and biological activity. Synthesized substances attract organic chemists with its high biological activity and low toxicity.

One of the important issues is the successful use of 1,2,3-triazole derivatives in agriculture and medicine against various diseases. In particular, based on 1,2,3-triazoles, drugs with high activity against microbes, cancer, inflammation, leishmania, tuberculosis, malaria. Research in the field of 1,2,3-triazoles began much earlier, and currently research based on compounds of this class is being carried out in many countries around the world. This can also be learned from articles that have been published in recent years in reputable journals.

The propargyl ester of disubstituted phenoxyacetic acid is a chemical compound that consists of a phenoxyacetic acid molecule with two substituents attached to the aromatic ring, and an ester group attached to the carboxyl group of the acid. Additionally, the ester group contains a propargyl functional group.

The solvents used were ethyl acetate, ethyl alcohol, hexane, acetone, benzene, and toluene. The structure of the synthesized compounds was reliably analyzed using modern IR, ¹H and ¹³C NMR spectroscopy. The progress of the reactions was monitored by thin layer chromatography (TCX). A mixture of hexane:ethyl acetate in a ratio of 3:1 was used as an eluent. The melting points of the synthesized compounds were determined in a MEL-TEMP device (USA).

The specific structure of the compound will depend on the nature of the substituents on the aromatic ring and the position of these substituents. The propargyl ester group is composed of a propargyl chain (CH≡C-) attached to the carboxyl carbon (C=O) of the phenoxyacetic acid moiety.

This compound may have potential applications in various fields such as organic synthesis, pharmaceuticals, or materials chemistry, depending on its specific properties and reactivity.

The exact characteristics of the propargyl ester of disubstituted phenoxyacetic acid will depend on the specific substituents on the aromatic ring and the position of these substituents. However, here are some general characteristics that can be associated with this compound:

1. **Reactivity:** The presence of the propargyl functional group makes this compound potentially reactive in various chemical reactions. The triple bond present in the propargyl group can undergo addition reactions, making it useful in a wide range of organic transformations.
2. **Stability:** Ester groups are generally stable under normal conditions, allowing for the compound to be handled and stored without significant degradation. However, the stability of the compound can be influenced by the nature of the substituents on the aromatic ring.
3. **Solubility:** The overall solubility of the compound will depend on the nature of the substituents on the aromatic ring and the ester group.

In a round-roll flask, 100 ml volume was added 0.595 g (0.005 mol) phenyluside, 0.66 g (0.005 mol) of the paro-hydroelectric monuro of monochloroacetic acid (1), 0.05 g (0.16 mmol) of iopid of copper (I) and 25.0 ml of toluene. The flask, equipped with reflux, was installed in a oil bath and heated at a boiling point of toluene (~ 110 ° C) for 6 hours. The progress of the reaction was controlled by thin layer chromatography. Over time, a yellow precipitate began to fall out of the reaction mixture. After 6 hours, the reaction was stopped and left at night at room temperature. Toluene was evaporated and the precipitate was recrystallized in hexane. The mass of the obtained product (2) 105 g, the output is 74%. MLP = 82- 84 ° C. RF 0.44 (System: Hexane: Ethyl acetate - 3: 1). 1N NMR (600 MHz, CDCl₃): 4.09 (2H, C, CL-CH₂-), 5.40 (2H, C, -OCO-CH₂-), 7.44 (1H, T, J = 7.43, AR-H-4), 7.52 (2H, T, J = 7.89, AR-H-3, 5), 7.71 (2H, D, AR-H- 2, 6), 8.09 (1H, C, Het-CH). 13C IMR (CDCl₃): 40.85, 59.11, 120.75, 122.72, 129.17, 129.93, 136.90, 167.47. IR spectrum (Kbr, v, CM⁻¹): 3153 (AR C-H), 3061 (C = C-H), 2960 (CH₂), 1751 (>C = O), 1636 (C = C), 1595 (n = n), 1501 (AR-NO₂), 1321 (C-O-), 1231 (Cn), 1173 (C-O-C).

The results obtained and their analysis. Analyzing the scientific literature published in recent years, we have set the target to synthesize the pro-graviter of monochloroacetic acid and conduct catalytic reactions of cycloprizzation with some aromatic azides. First, at the first stage, from the monochloroacetic acid and propagil alcohol, the corresponding propohygloratasetic ether (3) was synthesized. To remove water from the reaction medium, para-tululysulfonic acid (PTSC) was used. The resulting ether was thoroughly washed with water, dried and purified by distillation in vacuo.

When analyzing the IR spectrum of the substance 2, the corresponding frequency of absorption fluctuations characteristic of the aromatic carbon-rodent (AR C-H) are characterized, which are in the region 3153 cm⁻¹, for a carbon-hydrogen bond (C = C-H) in the triazole ring in the region 3061 cm⁻¹, for the carbonyl group (>C = O) is located in the region of 1751 cm⁻¹, for double carbon-carbon of the absorption frequency bonds are observed in the regions of 1231 cm⁻¹, while the corresponding fluctuations in the bonds of carbon-oxygen-carbon (C-O-C) had absorption frequencies in the region 1173cm⁻¹. The structure (1- (4-bromophenyl) -1H-1,2,3-triazol-4-yl) methyl 2-chloroacetatus (3) was also studied and analyzed by IRC, NMR spectra. According to the results of the resulting spectrum, complete compliance with substances of these structures was fully proved.

Synthesized derivatives of triazole are new compounds, and the biological activity of these substances is currently being studied. Conclusions by mutual esterification of monochlorocetic acid and propalygyl alcohol was synthesized by propagillachlaratasetate. The cyclassization reactions of the resulting propolyglychloroacetic ether with phenylzide and para-bromophenylosene was carried out. The catalysts of copper (I) were used as catalysts. The

greatest reaction output was achieved when iodide copper (i) was used. As a result, new derivatives of 1H-1,2,3-triazols in the 1,4-isomeric state (2, 3) were highlighted. These studies can be successfully applied in the future for the purpose of the reactions. The simplicity and convenience of these methods determine their advantages.

In the second stage, the cyclization of the propagillary chloroacetate was carried out by means of the Hysgen reaction. The necessary phenylacetic acid and pair bromophenyls are synthesized using the methods listed in the literature. The mutual reaction of synthesized propionylchloroacetate and aromatic amines was carried out. The cyclization response was carried out by heating the mixture of the reagents in a ratio of 1: 1 in the presence of a catalyst and a solvent. The catalysts (c) were used as catalysts. Toluene was used as a solvent. The reaction was carried out at a boiling point of toluene in the presence of different amounts of catalyst during the reaction.

The greatest yield of the reaction was achieved when iodide copper (I) was used as a catalyst, and the reaction was carried out at a boiling point of toluene for 6-8 hours. After the experiment, the reaction mixture was cooled, the toluene was removed by distillation, and the solid residual part was recrystallized from hexane. The dedicated substances were dried and studied by physical constants. The results showed that new 1,4-1,2,3-triazole (2-3) derived obtained with higher yields are obtained.

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