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LETTERS TO THE EDITOR

Synthesis of 2-Methyl-2-(3-phenoxybenzoyloxy)propionitrile

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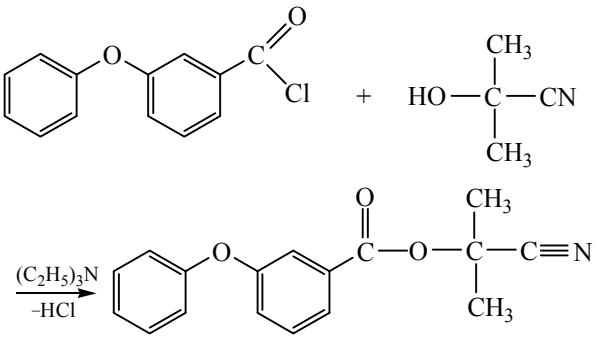
Nowadays the diphenyl oxide derivatives containing versatile functional groups are of significant practical interest. Many of them exhibit biomedical activity, and some of them are used in the agriculture. Of great interest in this series are nitriles, whose molecules contain in the side chain various functionalities alongside cyano group.

We developed an effective approach towards the synthesis of 2-methyl-2-(3-phenoxybenzoyloxy)propionitrile on the basis of 3-phenoxybenzoic acid chloride and acetone cyanohydrine which is 3-phenoxyphenyl-containing compound of the new structure. It can be of interest as an intermediate in the synthesis of biologically active compounds.

The incorporation of 3-phenoxyphenyl fragment in the pharmacophore molecule is a promising way to the synthesis of the new biologically active substances [1–4].

2-Methyl-2-(3-phenoxybenzoyloxy)propionitrile was obtained by the reaction of the 3-phenoxybenzoic acid chloride with acetone cyanohydrine in the anhydrous diethyl ether in the presence of triethylamine as the hydrogen chloride acceptor:



The synthesis was performed at room temperature (20–25°C) under stirring for 1 h using the 3-phenoxybenzoic acid chloride–acetone cyanohydrine–triethylamine in a molar ratio 1:1.2:1.2.

The structure and composition of the compound obtained was confirmed by IR and ^{1}H NMR spectroscopy.

2-Methyl-2-(3-phenoxybenzoyloxy)propionitrile. To a solution of 10 g (0.0462 mol) of 3-phenoxybenzoic acid chloride in 30 ml of anhydrous ethyl ether in a four-neck round-bottom flask equipped with a mechanical stirrer, a thermometer, a dropping funnel, and a reflux condenser bearing a calcium chloride tube was added dropwise 5.6 g (0.05544 mol) of triethylamine in 10 ml of anhydrous diethyl ether. Then to the reaction mixture was added dropwise 4.7124 g (0.05544 mol) of acetone cyanohydrine in 10 ml of anhydrous diethyl ether. The synthesis was performed under stirring at 20–25°C within 1 h. The triethylamine hydrochloride precipitate was filtered off, and the solvent was removed from the filtrate by distilling off first at atmospheric pressure and then in a vacuum. 2-Methyl-2-(3-phenoxybenzoyloxy)propionitrile was isolated by vacuum distillation. Yield 12.3 g (95%), a very viscous liquid of dark color, bp 190–192°C (3 mm Hg). ^{1}H NMR spectrum, δ, ppm: 1.8 s (6H, CH_3), 6.9–7.8 m (9H, $C_6H_5OC_6H_4$). IR spectrum, ν, cm^{-1}: 2224 (CN), 2938 (CH), 1287 (5CH_3), 1732 (C=O).

The IR spectrum was recorded on a Specord M-82 spectrophotometer (mull in mineral oil, NaCl or KBr prisms). The ^{1}H NMR spectrum was registered on a Varian Mercury 300BB spectrometer (DMSO-d_6), internal reference HMDS.

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