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Synthesis of benzyloxybenzyl derivatives of 2- и 4-(1*H*-azol-1-ylmethyl)phenols

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Abstract

The synthesis of 1-[2-(benzyloxy)benzyl]- and 1-[4-(benzyloxy)benzyl]-1*H*-azoles has been reported. These compounds were prepared from the corresponding 2- and 4-(1*H*-azol-1-ylmethyl) phenols in the presence of sodium hydride in anhydrous dimethylformamide. As the nitrogen component, nitrogen compounds with different nitrogen atoms in the cycle, their methylated and benzo-fused derivatives: imidazole, 2-methylimidazole, 1,2,4-triazole, benzimidazole, 2-methylbenzimidazole, benzotriazole were used. The structure of the compounds was confirmed by IR and ^{1}H NMR spectroscopy. The band of stretching vibrations of the hydroxyl group in the region 3135-2480 cm^{-1} in the IR spectra of 1-[2-(benzyloxy)benzyl]- and 1-[4-(benzyloxy)benzyl]-1*H*-azoles characteristic of azolylmethylphenols, the link is recorded in the form of several peaks in the 1260-1014 cm^{-1} region, which proves the presence of 2- and 4-(1*H*-azol-1-ylmethyl)phenols in the structure of the benzyloxybenzyl derivatives of the fragment (–$C_{аром.}$–O–C–). There are additional signals in the form of singlets in the range 5.12 ppm for *ortho*-derivatives and 5.14 ppm for *para*-derivatives, respectively, for 1-[2-(benzyloxy)benzyl]- and 1-[4-(benzyloxy)benzyl]-1*H*-azoles in the ^{1}H NMR spectra for the oxymethylene groups –CH_2O–. The ALOGPS 2.1 program was used to calculate the lipophilicity of both the obtained and the original compounds. All 1-[2-(benzyloxy)benzyl]- and 1-[4-(benzyloxy)benzyl]-1*H*-azoles, in contrast to 2- and 4-(1*H*-azol-1-ylmethyl) phenols are characterized by high lipophilicity. The lipophilicity of benzyl esters of 4- (1*H*-azol-1-ylmethyl) phenols is higher than that of 2-(1*H*-azol-1-ylmethyl)phenols, which is probably due to the greater spatial availability of the hydrophobic van der Waals surface in benzyl ester of 4-(1*H*-azol-1-ylmethyl)phenols. Methylated azole fragments, derivatives are also characterized by increased lipophilicity in comparison with their anmethylated analogues. The benzimidazole and benzotriazole derivatives were most lipophilic.

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