SYNTHESIS OF 2-ETHYNYLPYRIMIDINE

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Pyrimidines containing an unsubstituted acetylene group in position 2 are unknown. We have carried out the synthesis of 2-ethynylpyrimidine (I), which is a key compound in the synthesis of various acetylene derivatives of this series. Compound I was synthesized by decomposing 1-(2'-pyrimidyl)-3-methyl-1-butyn-3-ol (II) in the presence of KOH at 110°C under a residual pressure of 1.5 mm in Alkaren-2 vacuum oil with removal of the product from the reaction sphere [1]. The yield was 40%, and the product was in the form of white crystals, mp 95-96°C (from CCl_4). Compound I is soluble in water, ethanol, $CHCl_3$, and ether. Found: C 69.05; H 3.88; N 26.93%. Calculated for $C_6H_4N_2$: C 69.22; H 3.87; N, 26.91%. PMR spectrum ($CDCl_3$, δ, ppm): 3.07 (HC≡C), 7.20 (t, $H^{5'}$), 8.63 (H^4 and H^6). IR spectrum ($CHCl_3$, ν, cm^{-1}): 3320 v. s (HC≡C), 2135 v. s (C≡C). The original alcohol (II) was synthesized from 2-bromopyrimidine according to an acetylene condensation reaction [2, 3], the yield being 70%, and the mp being 78-79°C (C_6H_6—petroleum ether). Found: C 66.61; H 6.04; N 17.42%. Calculated for $C_9H_{10}N_2O$: C 66.65; H 6.21; N 17.27%. PMR spectrum ($CDCl_3$, δ, ppm): 1.60 (CH_3), 3.97 (OH), 7.20 (t, $H^{5'}$), 8.68 (d, $H^{4'}$ and $H^{6'}$). IR spectrum ($CHCl_3$, ν, cm^{-1}): 2258 s, 2225 (C≡C), 3603, 3380 br (OH).

LITERATURE CITED

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