REACTION OF 2-AMINO-3-ETHOXYCARBONYLTHIOPHENES WITH 2,3-DIBROMOPROPYL ISOTHIOCYANATE

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In the bromination of 4,5-dialkyl-2-(N-allylthioureido)-3-ethoxycarbonylthiophenes, a mixture difficult to separate is obtained. In the reaction of 4,5-dialkyl-2-amino-3-ethoxycarbonylthiophenes (I) with 2,3-dibromopropyl isothiocyanate, however, the closure not only of a thiazoline but also of a pyrimidine ring takes place, leading to a thieno[2,3-d]thiazolo[3,2-a]pyrimidine (II).

$$R \longrightarrow COOC_2H_5 + CH_2-CH-CH_2 \longrightarrow R \longrightarrow S \longrightarrow CH_2Br$$

$$I a.b \longrightarrow R - R = (CH_2)_4; b R = CH_3$$

2-Bromomethyl-2,3,4,5,6,7,8,9-octahydrobenzo[4,5]thieno[2,3-d]thiazolo[3,2-a]pyrimidin-5-one (IIa). A mixture of 4.5 g (0.02 mole) of 2-amino-3-ethoxycarbonyl-4,5,6,7-tetrahydrobenzo[b]thiophene (Ia) and 5.2 g (0.02 mole) of 2,3-dibromopropyl isothiocyanate in carbon tetrachloride was heated on the boiling water bath for 4 h. The precipitate was separated off and washed with ether. Yield 5.6 g (78%), mp 150-151°C (from methanol). UV spectrum (in ethanol, c 10^{-5} M), $\lambda_{\rm max}$, nm (log ϵ): 275 (3.09), 320 (3.27). Found: N 7.9; 7.7%. $C_{13}H_{13}{\rm BrN}_2{\rm OS}_2$. Calculated: N 7.8%.

2-Bromomethyl-6,7-dimethyl-2,3,4,5-tetrahydrothieno[2,3-d]thiazolo[3,2-a]pyrimidin-5-one (IIb) was obtained similarly from 2-amino-3-ethoxycarbonyl-4,5-dimethylthiophene (Ib). Yield 71%, mp 159-160°C (from methanol). UV spectrum (in ethanol, c 10^{-5} M), $\lambda_{\rm max}$, nm (log ϵ): 275(3,93), 325 (4.15). IR spectrum (molding with KBr): 1670 (C = O), 1310-1200 (CH₃), 660-540 (C-Br). Found: N 8.6; 8.5%. C₁₁H₁₁BrN₂OS₂. Calculated: N 8.5%.

The same bases (II) were obtained by decomposing the corresponding hydrobromides synthesized by an independent route [1].

LITERATURE CITED

1. V. Smolanka, A. A. Dobosh, and S. M. Khripak, Khim. Geterotsikl. Soedin., 1289 (1973).

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