Full Paper	Thematic Section: Preparative Chemistry.
Registration Code of Publication: 11-26-12-6	Subsection: Organic Chemistry

Publication is available for discussion in the Internet as a material of "All-Russian Working

Chemical Conference "Butlerov's Heritage-2011". http://butlerov.com/bh-2011/

Contributed to editorial board: July 29, 2011

Synthesis and iodocyclization of $3-((2E\{2Z\})-3-chloro-2-propenyl)$ thio-4-methyl-1,2,4-triazoles

© Elena S. Il'inykh, ** and Dmitry G. Kim*

Organic Chemistry Subdepartment. South Ural State University. Lenin St., 76. Chelyabinsk, 454080. Chelyabinskaya State. Russia. Phone: +7 (351) 265-95-70. E-mail: elena.ilinykh@mail.ru

Keywords: 3-mercapto-4-methyl-1,2,4-triazole, 3-((2E{2Z})-3-chloro-2-propenyl)thio-4-methyl-1,2,4-triazoles, 7-chloro-6-iodo-3-methyl-6,7-dihydro-5H-[1,2,4]triazolo[5,1-b][1,3]thiazinium iodide, iodocyclization, gas chromatography-mass spectrometry, ¹H NMR spectroscopy.

Abstract

In this paper, we report the interaction between 3-mercapto-4-methyl-1,2,4-triazole and 1,3-dichloropropene in alcohols in the presence of sodium alcoholates. By 1H NMR and mass spectra methods it was revealed that the reaction afforded the mixture of approximately equal amounts (1.00:1.00) of E- and Z-isomers of 3-(3-chloro-2-propenyl)thio-4-methyl-1,2,4-triazole. We found that the reaction of the synthesized S-alkenyl derivatives with iodine resulted in 7-chloro-6-iodo-3-methyl-6,7-dihydro-5H-[1,2,4]triazolo[5,1-h][1,3]thiazinium iodide being formed and its structure was investigated by 1H NMR.

6	© Butlerov Communications. 2011. Vol.26. No.12.	_ Kazan. Republic Tatarstan. Russia.

^{*}Supervising author; *Corresponding author