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2-Mercapto-5-(2'-isopropyl-5'-methylphenoxymethyl)-1,3,4-triazole

Abdullah Mohamed Asiri

Chemistry Department, Faculty of Science, King Abdul-Aziz University, Jeddah 21589, P.O. Box 80203, Saudi Arabia. Tel.(+696)-2-6952293, Fax (+696)-2-6952293, E-mail: a_asiri@hotmail.com

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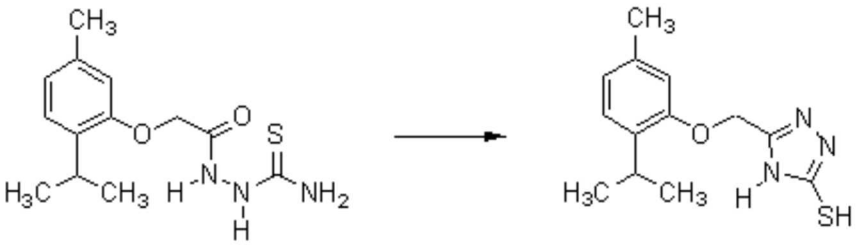

1 **2**

The triazole derivative **2** was prepared from 4-[2'-isopropyl-5'-methylphenoxyacyl]thiosemicarbazide **1** by heating under reflux with aqueous NaOH [1,2]. 4-[2'-Isopropyl-5'-methylphenoxyacyl]thiosemicarbazide **1** (1.0 g, 3.56 mmol) was suspended in aqueous NaOH (10 mL, 8%) and heated under reflux for 4 hours. The reaction mixture was treated with charcoal and filtered. The filtrate was cooled to room temperature and acidified carefully with dilute acetic acid (10%). The precipitate thus formed was filtered, washed with copious amount of water and recrystallized from ethanol to give **2** as white crystals (0.76 g, 81%).

Mp. 170-172°C (EtOH, uncorrected).

UV l_{max} (nm; Acetone)/e ($dm^3.mol^{-1}.cm^{-1}$): 331/4718.

IR (KBr): 3500 (NH), 2657 (SH), 1600 (C=N), 1575 (NH bending).

^{1}H-NMR (400 MHz; CDC_{l3}; Me_4Si): 1.20, 1.23 (6H, d, $2CH_3$), 2.31 (3H, s CH_3), 3.34 (1H, m, CH), 4.67 (2H, S, CH_2O), 6.56 (1H, s), 6.81 1H, d, *J* = 7.67 Hz), 7.12 (1H, d, *J* =7.70 Hz), 7.26 (1H, s, SH).

^{13}C-NMR (100 MHz; $CDCl_3$):21.27, 22.82, 26.6, 65.35 (CH_2O), 112.5, 122.77, 126.42, 134.57, 136.52, 154.58, 173.5(C-SH).

Anal.Calc. for $C_{13}H_{17}N_3OS$ (263.364): C 59.29, H 6.51, N 15.96; found : C 59.38, H 6.43 , N16.15.

References

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Sample availability: available from the authors and MDPI.