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5-[(2-isopropyl-5-methylphenoxy)methyl]-4-phenyl-4H-1,2,4-triazole-3-thiol

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5-[(2-Isopropyl-5-methylphenoxy)methyl]-4-phenyl-4*H*-1,2,4-triazole-3-thiol

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The triazole derivative **2** was prepared from 2-[(2-isopropyl-5-methylphenoxy)acetyl]-*N*-phenylhydrazine carbothioamide (**1**) by heating under reflux with aqueous NaOH [1,2]. **1** (1.0 g, 2.80 mmol) was suspended in aqueous NaOH (15 ml, 8%) and heated under reflux for 5 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 (0.81 g, 85%).

M.p. 165-167 °C (EtOH, uncorrected).

UV lmax (nm; Acetone)/e (dm³.mol⁻¹.cm⁻¹) 336/2900.

IR nmax (cm⁻¹; KBr Disk) 3450 (NH), 2657 (SH), 1612 (C=N), 1581 (NH bending).

¹H-NMR (400 MHz; CDCl₃; Me₄Si d_H) 1.08 (6H, d, 2CH₃), 2.27 (3H, s CH₃), 2.98 (1H, m, CH), 4.90 (2H, S, CH₂O), 6.57 (1H, s), 6.78 1H, d, J = 7.67 Hz), 7.07 (1H, d, J = 7.70 Hz), 7.46 (1H, s, SH), 7.53 (3H, m), 7.54 (2H, m).

¹³C-NMR (d_C) 21.65, 23.43, 26.2, 60.74, (CH₂O), 113.15, 123.2, 126.7, 128.2, 130.14, 130.6, 133.4, 134.96, 136.9, 149.08, 154.62, 169.78 (C-SH).

Elemental Analysis: Calculated for $C_{19}H_{21}N_3OS$ (339.22): C 67.27, H 6.19, N 12.39; found : C 67.12, H 5.96, N 12.13.

References

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