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4-(Benzylthio)acetophenone

Bruce A. Hathaway* and Mary M. Triefenbach

Department of Chemistry, Southeast Missouri State University, MS 6400, One University Plaza, Cape Girardeau, Missouri, 63701, USA. Tel. 001 573-651-2370; Fax 001 573-986-6433. E-mail: bahathaway@semovm.semo.edu

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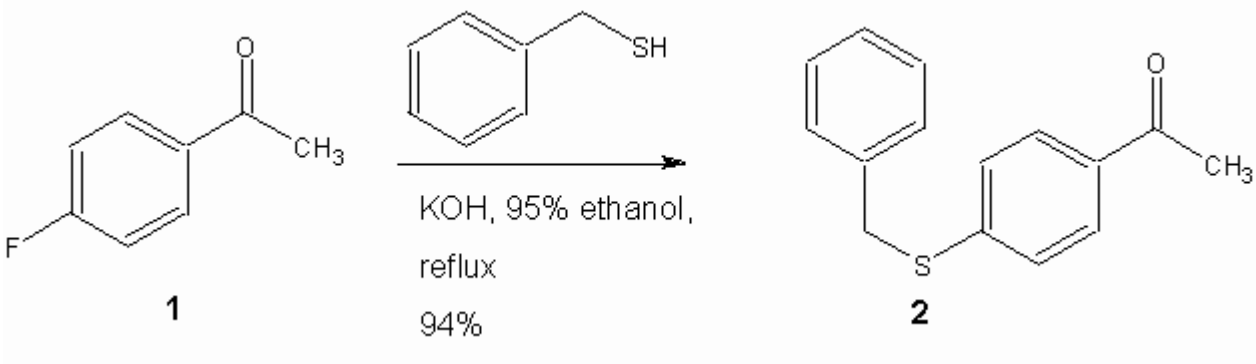

During the course of our research on preparing parallel dipole-aligned crystals [1-2], we needed to prepare the previously unreported compound 4-benzyl-sulfonylacetophenone. For this purpose we developed a two-step sequence via the title compound **2**, prepared in turn from commercially available 4-fluoro-acetophenone (**1**). Benzylmercaptan was dissolved in 95% ethanol, and converted to its potassium salt with KOH. It then was reacted with **1** to produce 4-(benzylthio)acetophenone (**2**) in high yield.

Benzylmercaptan (5.00 g, 40 mmol) was dissolved in 95% ethanol (20 mL). Potassium hydroxide (2.57 g, 40 mmol) was added. The resulting solution was heated to reflux until KOH had completely dissolved and was cooled to room temperature. 4-Fluoroacetophenone (5.58 g, 10 mmol) dissolved in 20 mL of 95% ethanol was then added dropwise. The solution was heated to reflux for 6 hours. When cooled, a solid precipitate formed, which was filtered and washed with 95% ethanol and water. The solid was dissolved in ether, washed with water and 1N NaOH aqeous solution, dried with $MgSO_4$, and the solvent removed to yield a white solid.

Yield: 9.18 g (94%).

Melting point: 110-112 ºC.

IR (KBr pellet, cm^{-1}): 2922, 1677, 1583, 1384, 1359, 1266, 1186, 1098, 817, 722, 695.

^{1}H-NMR (300 MHz, $CDCl_3$, ppm): 7.82 (2H, doublet, J=8.3 Hz), 7.30 (7H, multiplets), 4.20 (2H, singlet), 2.53 (3H, singlet).

^{13}C-NMR (75.5 MHz, $CDCl_3$, ppm): 198.61, 144.65, 136.64, 134.53, 129.17, 129.12, 127.95, 127.24, 37.52, 26.89.

MS (m/e, relative intensity): 91(100%), 65 (18%), 242 (M^+,15%); other peaks were <10%.

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References

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Sample availability: available from MDPI.