4-(Benzylthio)acetophenone

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Received: 28 May 2001 / Accepted: 14 December 2001 / Published: 20 December 2001

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-fluoroacetophenone (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 aqueous solution, dried with MgSO$_4$, and the solvent removed to yield a white solid.

Yield: 9.18 g (94%).

Melting point: 110-112 °C.

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%.

Acknowledgement: Acknowledgment is made to the donors of the Petroleum Research Fund, administered by the American Chemical Society, for partial support of this research.

References


*Sample availability:* available from MDPI.

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