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N-(3-Trifluoromethylphenyl)-4-nitroaniline

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The general part of the experimental section and the purposes of this synthesis have been present elsewhere [1]. A solution of 1,4-dinitrobenzene (168 mg, 1.00 mmol), 3-acetamidobenzotrifluoride (495 mg, 2.44 mmol) and tetrabutylammonium chloride (TBAC, 69 mg, 0.25 mmol) in chlorobenzene (ClBz, 5 mL) was stirred for 10 min at 70 °C. Then, 4 mL of 52.9 % w/w NaOH aqueous solution was added and the mixture was stirred for 16 hours at 70 °C. The mixture was neutralized with ammonium chloride solution, washed with water and extracted with dichloromethane. The organic phase was dried with MgSO4, filtered and the solvent removed under reduced pressure. Flash column chromatography (silica gel, chloroform) afforded 74 mg of the pure N-(3-trifluoromethylphenyl)-4-nitroaniline.

M.p. 123-124 °C.

TLC (silica gel, chloroform): R_f 0.26

FT-IR (KBr): 3382 (NH), 3092 (C_{Ar}-H), 1602, 1512 (NO₂), 1315 (NO₂), 1304, 1108.

¹HNMR (CDCl₃): 6.37 (bs, 1H, NH); 7.01 (d, 2H, J=8.7Hz); 7.44 (m, 4H), 8.17 (d, 2H, J=8.7Hz).

 $MS (m/z): 282.1 (M^{+}).$

Anal. Calcd. for C₁₃H₉F₃N₂O₂: C 55.33, H 3.21, N 9.93; found C 55.45, H 3.17, N 9.98.

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Reference

1. Durantini, E. N.; Chiacchiera, S. M.; Silber, J. J. Synth. Commun. 1996, 26, 3849-3858.

Sample Availability: Available from the authors.

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