

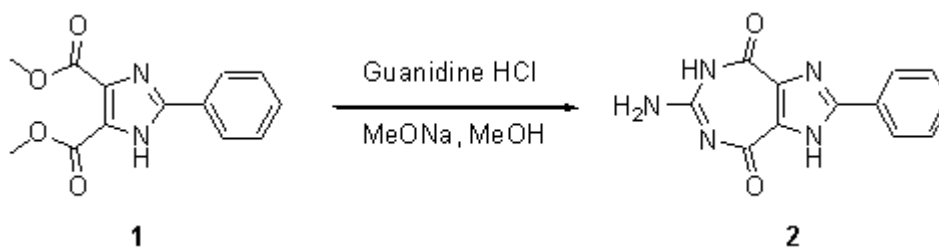
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6-Amino-2-phenylimidazo[4,5-*e*][1,3]diazepine-4,8(1*H*, 5*H*)-dione

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The starting imidazole diester (**1**) was prepared by esterification of the corresponding dicarboxylic acid according to the literature procedure [1,2]. A solution of dimethyl 2-phenyl-1*H*-imidazole-4,5-dicarboxylate (**1**) (0.26 g, 1 mmol) and guanidine hydrochloride (0.48 g, 5 mmol) in 50 mL of absolute methanol was stirred for 30 min at room temperature, then 2 mL of 25% sodium methoxide solution in methanol was added. The resulting mixture was stirred for 48 h at room temperature. The precipitate formed was filtered and washed with methanol to give sodium salt of the product as a white solid. The sodium salt was dissolved in water and neutralized with 2 M hydrochloric acid to yield the title compound (**2**) as a white solid after filtration and washing with water, yield 0.21 g (78%).

M.p. >260 °C.

TLC (CHCl₃: MeOH: 30% NH₄OH, 2:2:1): R_f 0.61.

¹H NMR (DMSO-*d*₆): 13.74 (br s, 1H, NH, exchangeable with D₂O), 10.68 (br s, 1H, NH, exchangeable with D₂O), 8.20 (m, 2H, Ph), 7.60 (br s, 1H, NH, exchangeable with D₂O), 7.48 (m, 3H, Ph), 6.50 (br s, 1H, NH, exchangeable with D₂O).

FABMS: 256 [MH⁺].

Anal. Calcd. for C₁₂H₉N₅O₂·3/4H₂O (268.75): C, 53.63; H, 3.94; N, 26.06. Found: C, 53.62; H, 4.02; N, 26.03.

References

1. Anderson, W. K.; Bhattacharjee, D.; Houston, D. M. *J. Med. Chem.* **1989**, *32*, 119-127.
2. Manecke, G.; Schlegel, R. *Chem. Ber.* **1974**, *107*, 892-897.

Sample availability: available from the authors and from MDPI (MDPI ID 18548).

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