

Short Note

4,6-Diamino-5-(4-methylbenzylidene)pyrimidin-2(5H)-one

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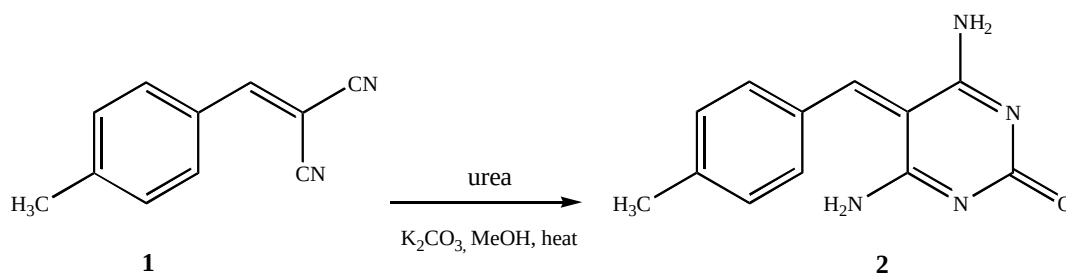
Received: 26 November 2009 / Accepted: 11 December 2009 / Published: 27 January 2010

Abstract: A new compound, 4,6-diamino-5-(methylbenzylidene)pyrimidin-2(5H)-one, was synthesized and its IR, ¹H NMR, ¹³C NMR and MS spectroscopic data are presented.

Keywords: 4,6-diamino-5-(4-methylbenzylidene)pyrimidin-2(5H)-one; urea; antimicrobial activity

Pyrimidines and their derivatives are considered an important group of compounds because of the diversity of biological activities associated with these systems. Among the activities reported for pyrimidines have been found antifolate [1], antimicrobial [2], leishmanicidal [3], anticonvulsant [4], anti-rubella [5], anti-HIV [6], calcium channel modulation [7], and selective hepatitis B virus inhibition [8].

In the specialized literature, we can find different articles on the synthesis of substituted pyrimidines and many detailed reviews have appeared [9–12]. Recently, the Biginelli reaction is a well-known multicomponent reaction involving a one-pot cyclocondensation of an aldehyde, a methylene active compound and urea/thiourea for the synthesis of pyrimidine derivatives [13–15]. Nevertheless, little attention is given to the synthesis and biological activity of the pyrimidine nucleus having the benzylidene group in position 5, close to amino groups at positions 4 and 6. We report here the synthesis and biological activity of 4,6-diamino-5-(4-methylbenzylidene)pyrimidin-2(5H)-one **2**.



A mixture of (4-methylbenzylidene)malononitrile **1** [16–18] (0.2 g, 1.19 mmol), urea (0.14 g, 2.33 mmol), and K_2CO_3 (0.20 g, 1.17 mmol) in methanol was refluxed for 24 h. The reaction mixture was neutralized with HCl (10% v/v). The solid was filtered and washed with water. After recrystallization using methanol, 4,6-diamino-5-(4-methylbenzylidene)pyrimidin-2(5H)-one **2** was obtained as a brown solid (0.18 g, 80%). Synthesis of other pyrimidine derivatives and studies of their biological activities are in progress, mainly tests of antimicrobial activity as a part of a research program directed to the synthesis of novel heterocyclic compounds of pharmacological interest.

M.p.: 172–175 °C.

IR (KBr, cm^{-1}): 3271 (NH_2), 1780 (C=O), 1651 (C=N).

^1H NMR (CDCl_3 , 270 MHz): δ : 8.34 (1H, s, olefinic-H); 7.89 (2H, dd, $J = 8.9, 2.0$ Hz, Ar-H); 7.18 (2H, dd, $J = 8.9, 2.0$ Hz, Ar-H); 4.91 (4H, br, NH_2); 2.30 (3H, s, CH_3).

^{13}C NMR (CDCl_3 , 69 MHz): δ : 160.02; 156.61; 144.07; 139.07; 132.28; 130.89; 129.02; 128.16; 21.17.

EI, MS (m/z , %): 228 (M^+ , 29%); 213 ($\text{M}^+ - \text{CH}_3$); 168 ($\text{M}^+ - \text{CO-N}_2\text{H}_4$, 100%).

Anal. Calcd for $\text{C}_{12}\text{H}_{12}\text{N}_4\text{O}$: C, 63.07%; H, 5.26%; N, 24.53%. Found: C, 63.47%; H, 5.41%; N 24.87%.

Biological Activity: Compound **2** showed antimicrobial activity against *Escherichia coli* (ATCC 35218) (ATCC 25922) (gram negative bacteria).

Acknowledgements

We are grateful to “Consejo de Desarrollo Científico y Humanístico de la Universidad Central de Venezuela /CDCH-UCV)” for financing the Project: **PI 06-00-6759-2007**.

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