Short Note

Synthesis and Characterization of N,N’-(propane-1,2 diydicarbamothioyl)dibenzamide

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Benzoylthioureas have found some interest due to their biological activity [1], spectroscopic and structural properties [2,3], or as synthetic building blocks [4]. Here, we report the convenient
preparation of a new representative of this type of compounds. Benzoyl isothiocyanate (1) was prepared by known methods reported in the literature [5]. Benzoyl isothiocyanate (21 ml) was added to a solution of 1,2-diaminopropane (17 ml) in anhydrous acetone. The resulting mixture was refluxed for 6 h. Finally, the mixture was cooled in an ice bath and 1M HCl (250 ml) was added. The yellow precipitate was collected by filtration and it was washed with diethyl ether. The title compound 2 thus obtained was recrystallized from EtOH/\(\text{CH}_2\text{Cl}_2\).

**Scheme 1.** \(^1\text{H}\) NMR spectrum of 2.

Color: yellow.

\(\text{Mp} \ 162-163^\circ\text{C}.

Elemental analysis: Found: C, 57.5; H, 5.1; N, 13.9; S, 16.0. Calc. for C\(_{19}\)H\(_{20}\)N\(_4\)S\(_2\)O\(_2\): C, 57.0; H, 5.0; N, 14.0; S, 16.0.

\(^1\text{H}\) NMR: \(\delta\) (CDCl\(_3\), 400.1 MHz): 11.00 (s, 1H, NH-CO); 10.96 (d, 1H, NH-CO); 9.04 (s, 1H, NH); 8.99 (s, 1H, NH); 7.84–7.52 (m, 10H, PhH); 5.03–4.98 (m, 1H, CH); 4.19–3.99 (m, 2H, CH\(_2\)); 1.46–1.44 (d, 3H, CH\(_3\)).

\(^{13}\text{C}\) NMR: \(\delta\) (CDCl\(_3\), 100.0 MHz): 185.2 (C=S); 164.0 (C=O); 135.6–127.2 (C=C\(_{\text{arom}}\)); 47.5 (CH); 46.9 (CH\(_2\)); 18.7 (CH\(_3\)).

IR (KBr) \(\nu_{\text{max}}/\text{cm}^{-1}\): 3350–3300 (N-H), 3161 (C-H\(_{\text{aromatic}}\)), 3038 (CH\(_3\)), 2935–2859 (C-H\(_{\text{aliphatic}}\)), 1980–1835 (C=C), 1677 (C=O), 1540–1258 (C-N), 1189, 1162 (C=S).
UV-vis (CH$_2$Cl$_2$, abs): 240; 400.

Table 1. Thermal analysis of 2.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Stage</th>
<th>TG results temperature range (°C)</th>
<th>DTA results temperature peak (°C)</th>
<th>Weight loss (%) Found/Calculated</th>
<th>Evolved moiety</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>I</td>
<td>180–240</td>
<td>226.71</td>
<td>43.684/44.75</td>
<td>C$_6$H$_5$CONHCSNH</td>
</tr>
<tr>
<td></td>
<td>II</td>
<td>240–340</td>
<td>282.56</td>
<td>44.884/44.75</td>
<td>C$_6$H$_5$CONHCSNH</td>
</tr>
</tbody>
</table>

References


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