

## 3-(2-Oxopropyl)-2(3H)-benzoxazolone

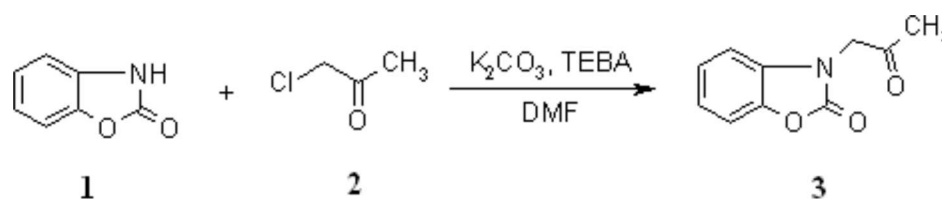
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The title compound is an important intermediate for the preparation of 3,4- and 3,4,5-substituted 1-(2-hydroxy-phenyl)imidazolin-2-ones [1, 2] and 6-methyl-4-(2-hydroxyphenyl)-1,2,4-triazin-3-ones [3]. According to literature data, the product 3 is prepared from 2(3H)-benzoxazolone with commercially unavailable bromoacetone in abs. ethanol in the presence of sodium ethoxide [4, 5]. We present an improved method for the synthesis of 3-(2-oxopropyl)-2(3H)-benzoxazolone (3) from available starting materials 1 and 2 under PTC conditions in higher yield.

To a mixture of 2(3H)-benzoxazolone (6.75 g, 50 mmol), fine powdered potassium carbonate (4.14 g, 30 mmol) and TEBA (200 mg) in DMF (15 ml), chloroacetone (4 ml, 50 mmol) was added. The reaction mixture was stirred for 1 h at 20–25 °C and then poured under stirring into 150 ml of water. The resulting precipitate was filtered and washed with water. Recrystallization from ethanol gave the product 3 as colorless needles. Yield: 90%.

Melting point: 119–120 °C

Elemental Analysis: Calculated for C<sub>10</sub>H<sub>9</sub>NO<sub>3</sub>: C 62.82%, H 4.74%, N 7.33%. Found: C 62.95%, H 4.53%, N 7.17%.

IR (nujol, cm<sup>-1</sup>): 1770, 1720 (CO).

<sup>1</sup>H-NMR (250 MHz, CDCl<sub>3</sub>): 2.25 (s, 3H, CH<sub>3</sub>); 4.61 (s, 2H, CH<sub>2</sub>); 6.77–7.21 (m, 4H, arom. H).

<sup>13</sup>C-NMR (63 MHz, CDCl<sub>3</sub>): 26.9 (CH<sub>3</sub>CO); 50.7 (CH<sub>2</sub>CO); 108.2 (C7); 109.9 (C4); 122.7 (C5); 123.8 (C6); 142.4 (C7a); 154.3 (C2); 199.8 (CH<sub>2</sub>CO).

MS (m/z, %): 191 [M<sup>+</sup>] (47); 148 (67); 120 (12); 104 (11); 77 (100); 65 (10); 50 (19).

### References

- Lozanova, Ch.; Kalcheva, V.; Simov, D. *Khim. Geterosikl. Soedin.* **1988**, *10*, 1362.
- Lozanova, Ch.; Kalcheva, V. *J. Prakt. Chem.* **1989**, *331*(6), 1007.

3. Bojtscheva, Ch.; Simov, D.; Kaltscheva, V. *J. Prakt. Chem.* **1979**, *321*(2), 226.
4. Zinner, H.; Randow, F. *J. Prakt. Chem.* **1961**, *4*, 144.
5. Simov, D. A.; Kalcheva, V.B.; Boycheva, H.S. *Compt. Rend. Acad. Bulg. Sci.* **1974**, *27*, 1073.

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