Crystal structure of methyl 3-(1,3-dioxo-1H-benzo[de]isoquinolin-2(3H)-yl)propanoate, C₁₆H₁₃NO₄

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains a list of the atoms including atomic coordinates and displacement parameters.

Source of material
All chemicals were purchased from commercial sources and used as received without further purification. The 3-(1,3-dioxo-1H-benzo[de]isoquinolin-2(3H)-yl)propanoic acid (5 mmol, 1.345 g) were dissolved in MeOH (50 mL), then two drops of 98% H₂SO₄ were added. The mixture was refluxed for 5 h. When the reaction vessel had cooled to room temperature, the reaction mixture was filtered.
The crystals of the title compound were obtained by controlled solvent evaporation.

**Experimental details**

All H-atoms bonded to C atoms were placed geometrically and refined using a riding model with common isotropic displacement factors $U_{iso}(H) = 1.2$ or $1.5 U_{eq}$(parent C-atom).

**Comment**

Alerstatin acting as aldose reductase inhibitors has been developed for the treatment of secondary complications in diabetes [5, 6], but has been withdrawn because of adverse effects [7]. The title compound is an important intermediate in the derivatization of alerstatin, so the synthesis and crystal structure of it is of great significance to study the reduction of side effects.

Single-crystal structure analysis revealed that the title compound crystallized in the monoclinic space group $P2_1/c$. The molecular title structure is presented in the Figure. The bond lengths of C15=O3, C11=O1, and C12=O2 in the title molecule are 1.195(2) Å, 1.219(2) Å, and 1.219(2) Å, respectively. They are similar to reported in the literature [8, 9]. It illustrated characteristic C=O double bonds. In addition, the bond length of N1–C11, N1–C12, N1–C13 in the title molecule are in the range of 1.398–1.476 Å. The bond lengths within the aromatic ring as well as C13–C14 and C14–C15 ones are close to their normal values.

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**References**