Crystal structure of (E)-N‘-(4-((E)-3-(dimethylamino)acryloyl)-3-hydroxyphenyl)-N, N-dimethylformimidamide, C$_{14}$H$_{19}$N$_{3}$O$_{2}$

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

In our research on the identification of anti-rot genes of pinellia ternata in Guizhou Province, we selected the hydroxyl aromatic ketonether derivate present in pinellia ternata as the raw material to synthesize the title compound. 1-(4-amino-2-hydroxyphenyl)ethan-1-one (3.02 g, 20 mmol) and dimethylformamide dimethylacetal (9.0 mL) were combined. The colorless solution heated to 383 K. Thin layer chromatography tracked the progress of the reaction until the 1-(4-amino-2-hydroxyphenyl)ethan-1-one is complete and the reaction is over. Then the reddish brown solution precipitated red solid when cooled to room temperature. The mixture was filtered and concentrated in vacuo to afford a solid. The solid was recrystallized from ethanol.

2 Experimental details

The carbon-bound hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

3 Comment

Enaminone compounds and their derivatives are widely used in the field of organic chemistry, pharmaceutical chemistry, which are used as intermediates to synthesize many active drugs [4, 5]. Some enaminone compounds can be used as potential anticonvulsants and as potential multidrug resistance regulator [6–8]. In the field of anti-inflammatory and antiepileptic drug research, they play an important role [9]. In addition, in our research of the identification of antiseptic genes of pinellia, an important national Chinese medicinal material, adopting functional genomics approach, collecting pinellia fine medicinal materials from Hezhang, Dafang, and other places in Guizhou Province, China. We find that enaminone compounds are
also present in Guizhou’s pinellia ternata. Enaminone compounds are also used as raw material to synthesize flavonoids in pinellia ternata. Therefore, the synthesis and modification of enaminone compounds has been a hot topic. The structure of the title compound is a kind of enaminone, containing a benzene ring, a hydroxyl group, a ketone and two enamines. The bond lengths and angles derived from the title structure are within normal ranges [10, 11]. The keto group was confirmed by the distance of 1.2664(17) Å (C7–O1), the phenolic hydroxyl was confirmed by the distance of 1.3520(17) Å (C1–O2), the C8–C9 double bond adopts an E-configuration and the bond distance is 1.365(2) Å, the bond distance of the N2=C12 double bond is 1.289(2) Å. The torsion angles of O2–C1–C2–C3 and N2–C3–C4–C5 are –179.04(14)° and –175.56(15)°, respectively.

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**References**


