TGA/DSC was applied to determine the decomposition temperature, melting temperature \((T_m)\) and fusion enthalpy \((\Delta_{fus}H)\). The results are graphically shown in Figure S1. As shown in the DSC curve, a strong endothermic melting peak shows that isatoic anhydride melts at 515.65 K, which is close to the values reported by Klenov et al. and Zheng et al. However, the TGA curve indicates that the melting process is accompanied with an obvious decomposition of the sample. Therefore, the general thermal analysis method cannot obtain the accurate melting temperature and fusion enthalpy of isatoic anhydride.
In order to obtain the melting temperature and fusion enthalpy of the compound, Akash Jain et al. proposed a method for estimating the normal melting temperature in combination with additive group contributions and non-additional molecular parameters. The model was applied to more than 2,200 compounds, including some drugs with complex structures, given an average absolute error of 30.1 K, which is relatively small considering the wide range of related organic compounds. According to the model, the melting temperature and fusion enthalpy can be estimated by the following equation:

$$T_m = \frac{\Delta_{fus}H}{\Delta_{fus}S}$$

$$\Delta_{fus}H = \sum n_i m_i + \sum n_j m_j$$

$$\Delta_{fus}S = 50 - 8.314\ln \sigma + 7.382\tau$$

$$\tau = SP3 + 0.5SP2 + 0.5RING - 1$$

where $\Delta_{fus}H$ and $\Delta_{fus}S$ represent the fusion enthalpy and fusion entropy, respectively; $n_i$ and $n_j$ represent the number of times that group i and proximity factor j appear in a compound, respectively; $m_i$ and $m_j$ represent the corresponding contribution to the fusion enthalpy. $\sigma$ stands for the rotational symmetry number, $\tau$ is flexibility number or the effective number of torsional angles. SP3 is the number of nonring, nonterminal sp$^3$ atoms such as CH$_2$, CH, C, NH, N, O, and S, SP2 is the

Figure S1. TGA/DSC curve of isatoic anhydride.

![TGA/DSC curve of isatoic anhydride](image.png)
number of nonring, nonterminal sp$^2$ atoms such as =CH, =C, =N, and C=O, and RING represents the number of single or fused aromatic ring systems.