Coumarin derivative, 7-hydroxy-3-(4-nitrophenyl)-coumarin (C15H9N1O5) was synthesized by knoevenagel condensation reaction by using 2,4-Dihydroxybenzaldehyde and 4-nitrophenylacetonitrile. The title compound was characterized by FT-IR, NMR and LCMS spectral studies and finally, the structure was confirmed by X-ray diffraction studies. The crystal structure of the title compound displays a two-dimensional architecture. The compound exhibits both inter and intra-molecular hydrogen bonds of type O—H…O and C—H…O. In addition, DFT calculations and Hirshfeld surface analysis were carried to analyze nature of hydrogen bonding, inter-molecular interaction in crystal, and to examine the molecular shapes. The overlapping of atomic orbital along with their predicted energy is explained on the basis of HOMO-LUMO energy gap calculations. Molecular electrostatic potential map was studied for predicting the reactive sites.


**Keywords:** Coumarin derivative, X-ray diffraction, Hirshfeld surface

**Figure:** (a) Molecular structure and (b) intermolecular interactions of the title compound.