Synthesis, Crystal structure and Hirshfeld surface analysis of a novel chalcone derivative: (2E)-3-(2,3-dimethoxyphenyl)-1-(3-nitrophenyl)prop-2-en-1-one

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Abstract

A novel chalcone derivative (2*E*)-3-(2,3-dimethoxyphenyl)-1-(3-nitrophenyl)prop-2-en-1-one (3DPNP) has been synthesized and crystals have been grown by slow solvent evaporation solution growth technique. The crystals were characterized by FTIR, ^{1}H NMR, DSC, TGA and single crystal X-ray diffraction methods. The crystals are thermally stable up to 143.5°C. The compound crystalizes in the monoclinic system, in centrosymmetric space group $P2_1/n$ with unit cell parameters a =8.6125(3) Å, b =12.3005(4) Å, c =14.8416(5) Å, α = γ = 90.00°, β =103.97(2)°, Z = 4, V =1525.79(9) Å^3. The C–H…O intermolecular hydrogen bonding interactions stabilizes the crystal structure. Further the Hirshfeld surface analysis facilitates the study of the nature of intermolecular interactions and fingerprint plots provide the information about the percentage contribution from each individual contact.

Keywords: Crystal structure, Chalcones, X-ray diffraction, Hirshfeld surface analysis, Fingerprint plots.

Specifications Table

Subject area	*Organic Chemistry, X-ray crystallography*
Compounds	(2*E*)-3-(2,3-dimethoxyphenyl)-1-(3-nitrophenyl)prop-2-en-1-one