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Methyl (*E*)-3-(5-cyano-2-furyl)-2-phenylacrylate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.058
wR factor = 0.139
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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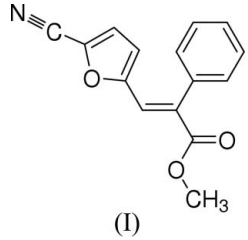
In the title compound, $C_{15}H_{11}NO_3$, the dihedral angle between the mean planes of the furan and phenyl rings is 64.7 (1)°. The molecules are linked into infinite chains by C—H···O and C—H···π interactions.

Comment

Cyano-substituted compounds are the precursors for the synthesis of diverse amidino derivatives, which have a broad spectrum of biological activities (Tidwell *et al.*, 1990; Patrick *et al.*, 1997; Hranjec *et al.*, 2003; Jarak *et al.*, 2005). The title compound, (I), is an intermediate in the synthesis of an acyclic amidino derivative (DNA inactive) that can be efficiently converted by UV irradiation into its cyclic naphthofuran derivative (DNA active), which offers a new attractive approach to photoinduced anticancer therapy (Starčević *et al.*, 2005). As a part of a study on the synthesis and biological activities of cyano- and amidino-substituted furyl–phenyl acrylates, the synthesis of cyano derivative (I) was carried out (Starčević *et al.*, 2006) and its structure is presented here.



(I)

The characteristic feature of (I) (Fig. 1) is a π-conjugated system extended over almost the entire molecule, excluding the phenyl ring. The phenyl and furan rings form dihedral angles of 65.8 (2)° and 11.3 (2)°, respectively, with the plane defined by atoms C4, C6, C7 and C8. The dihedral angle between the mean planes of the furan and phenyl rings is 64.7 (1)°.

The molecules of (I) are linked by C3—H3···O2($1+x, \frac{1}{2}-y, \frac{1}{2}+z$) intermolecular hydrogen bonds between the furan ring and the ester group (Fig. 2; Table 1), generating a *C*(7) chain motif (Bernstein *et al.*, 1995). This chain is additionally stabilized by C—H···π interactions between the furan H2 atom and the phenyl ring (Fig. 2; Table 1).

Experimental

The synthesis of compound (I) was described by Starčević *et al.* (2006). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a petroleum ether solution at room temperature.

Crystal data

$C_{15}H_{11}NO_3$
M_r = 253.25
Monoclinic, $P2_1/c$
a = 6.2701 (5) Å
b = 19.948 (2) Å
c = 10.672 (1) Å
β = 102.180 (8)°
V = 1304.8 (2) Å^3
Z = 4
D_x = 1.289 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, colourless
0.46 × 0.41 × 0.38 mm

Data collection

Oxford Diffraction Xcalibur2 diffractometer
ω scans
Absorption correction: none
16533 measured reflections
3138 independent reflections
2918 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 28.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.139
S = 1.12
3138 reflections
205 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.3164P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.93 (2)	2.54 (2)	3.121 (2)	120 (1)
C2—H2···Cg^{i}	0.98 (2)	2.65 (2)	3.566 (2)	156 (2)

Symmetry code: (i) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$.

H atoms of the methyl group were placed in calculated positions with C—H = 0.96 Å and with U_{iso}(H) = 1.5U_{eq}(C). Torsional parameters of the methyl group were refined. All other H atoms were found in a difference Fourier map and their coordinates and isotropic displacement parameters were refined freely [C—H = 0.93 (2)–0.98 (3) Å].

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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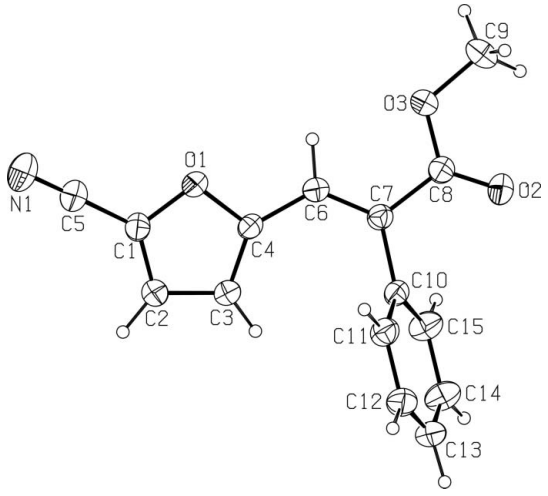

Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

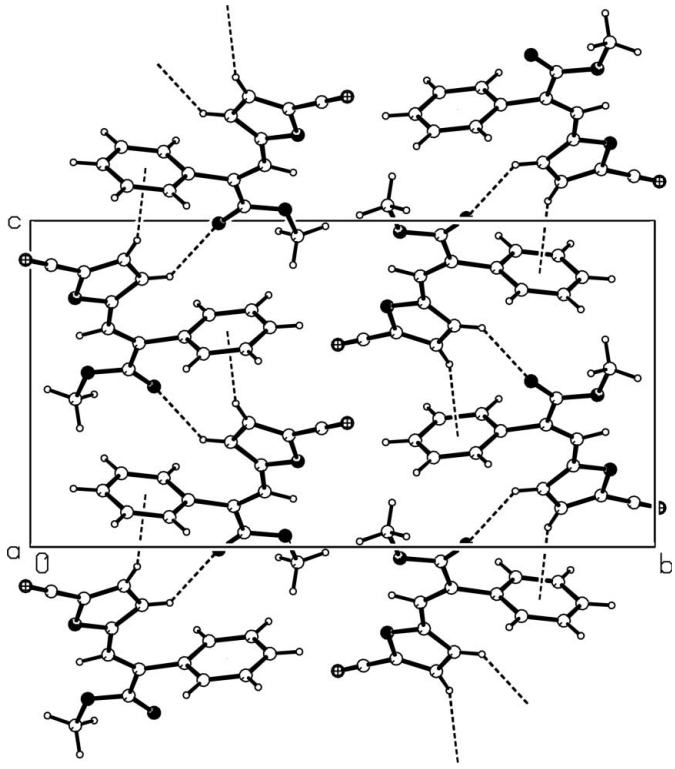

Figure 2
The crystal packing of (I), viewed along [100], showing infinite chains formed by C—H···O and C—H···π interactions (indicated as dashed lines).

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