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Ethyl 2,5-diphenylfuran-3-carboxylate

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In the title compound, $C_{19}H_{16}O_3$, the dihedral between the two phenyl rings is 12.6 (1)°. An intramolecular hydrogen bond and weak $C—H\cdots\pi$ interactions are observed.

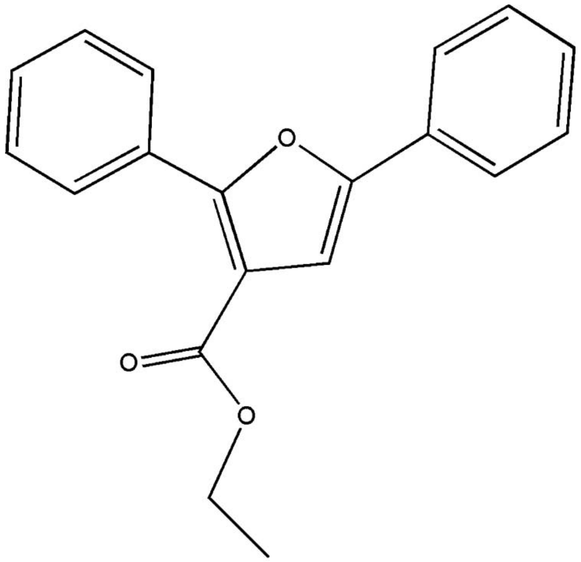
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.119
Data-to-parameter ratio = 16.9

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

Comment

Recently, we have reported the structure of diethyl 2,5-bis(3,4,5-trimethoxyphenyl)furan-3,4-dicarboxylate (Hu & Wu, 2005). In order to study the influence of the methoxy and ethyl groups on the packing of the crystal structure, we have synthesized the title compound, (I), which has an analogous molecular structure.



(I)

In the molecule, the dihedral angle between the two phenyl rings is 12.6 (1)° (Fig. 1), larger than the value of 8.8 (1)° in the diethyl compound (Hu & Wu, 2005). Analysis of the reported atomic coordinates using *PLATON* (Spek, 2003) shows that intermolecular hydrogen bonds are absent in the crystal structure of (I); however, the molecules are weakly linked together by three $C—H\cdots\pi$ hydrogen bonds involving one Csp^2 and two Csp^3 atoms (Fig. 2 and Table 1).

Experimental

The title compound, (I), was synthesized according to the literature procedure of Wu *et al.* (1997). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature.

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Crystal data

$C_{19}H_{16}O_3$
$M_r = 292.32$
Orthorhombic, *Pbca*
$a = 9.6272$ (9) Å
$b = 15.0692$ (14) Å
$c = 21.2860$ (19) Å
$V = 3088.1$ (5) Å^3
$Z = 8$
$D_x = 1.258$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 5225 reflections
$\theta = 2.3$–$25.1°$
$\mu = 0.08$ mm^{-1}
$T = 292$ (2) K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART Apex CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.975$, $T_{\max} = 0.992$
17087 measured reflections

3375 independent reflections
2544 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\max} = 27.0°$
$h = -10 \rightarrow 12$
$k = -19 \rightarrow 18$
$l = -22 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.119$
$S = 1.03$
3375 reflections
200 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 0.433P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 phenyl and furan rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2	0.93	2.17	3.001 (2)	148
C13—H13···*Cg*1$^{\rm i}$	0.93	3.26	3.981 (1)	136
C18—H18*B*···*Cg*1$^{\rm ii}$	0.97	3.01	3.837 (1)	144
C19—H19*C*···*Cg*2$^{\rm ii}$	0.96	2.91	3.786 (1)	153

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

All H atoms were placed at their idealized positions (methyl C—H = 0.96 Å, methylene C—H = 0.97 Å and aromatic C—H = 0.93 Å) and included in the refinement in the riding-model approximation, with $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(C) for methyl H atoms and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) for methylene and aromatic H atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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: *PLATON*.

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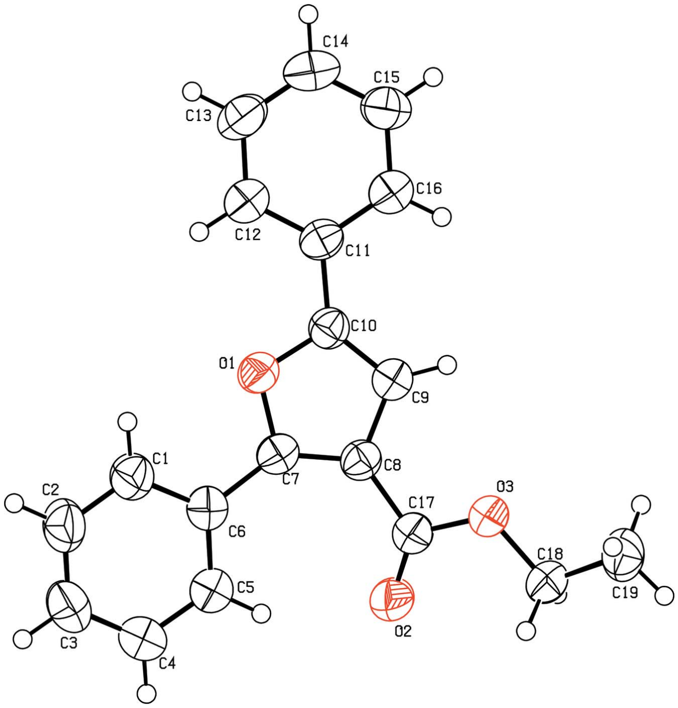

Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

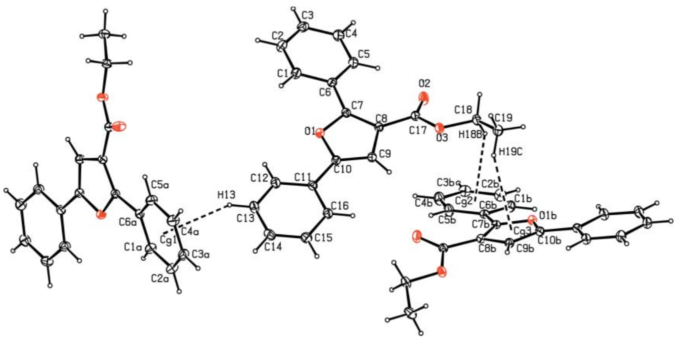

Figure 2
The linkage of the molecules by C—H···π interactions (dashed lines) [symmetry codes: (*a*) $2-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (*b*) $-\frac{1}{2}+x, \frac{1}{2}-y, 1-z$].

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