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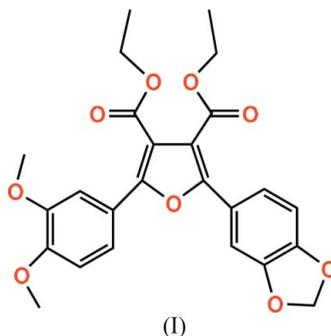
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chwuax@mail.ccn.u.edu.cn**Key indicators**Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.045
 wR factor = 0.126
Data-to-parameter ratio = 14.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**Diethyl 2-(1,3-benzodioxol-5-yl)-5-(3,4-dimethoxyphenyl)furan-3,4-dicarboxylate**

In the title compound, $\text{C}_{25}\text{H}_{24}\text{O}_9$, the substituted benzene rings are twisted away from the furan ring. The dihedral angle between the two benzene rings is $52.1(1)^\circ$. In the crystal structure, the molecules exist as hydrogen-bonded dimers, the molecules being connected through very weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Comment

Furan-3,4-dicarboxylic acid and its esters have been used as starting materials in the synthesis of several bioactive natural products and several pharmacologically useful compounds, in the preparation of complexes with rare earth metal ions, and also as potential dienes in Diels–Alder reactions for the synthesis of several novel heterocycles (Deshpande *et al.*, 2002). As part of a study of their applications, we report here the crystal structure of the title compound, (I).



In compound (I), the furan ring is planar and the two substituted benzene rings are twisted away from it (Fig. 1). The $\text{C}12/\text{C}13/\text{C}14/\text{C}16/\text{C}18/\text{C}19$ and $\text{C}2-\text{C}7$ benzene rings form dihedral angles with the furan ring of $39.5(2)$ and $23.4(1)^\circ$, respectively. The dihedral angle between the two benzene rings is $52.1(1)^\circ$. The $\text{C}2-\text{C}7$ aromatic ring is effectively coplanar with the five-membered $\text{C}1/\text{O}1/\text{C}2/\text{C}3/\text{O}2$ ring, as seen in the dihedral angle between their planes of $1.6(1)^\circ$. The conformation of the two substituted ester groups with respect to the central furan ring are different (see Table 1 for torsion angles). The crystal packing shows that the molecules exist as hydrogen-bonded dimers, the molecules being connected through very weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2). The dimers are interlinked also through very weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Fig. 2).

Experimental

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 298 K.

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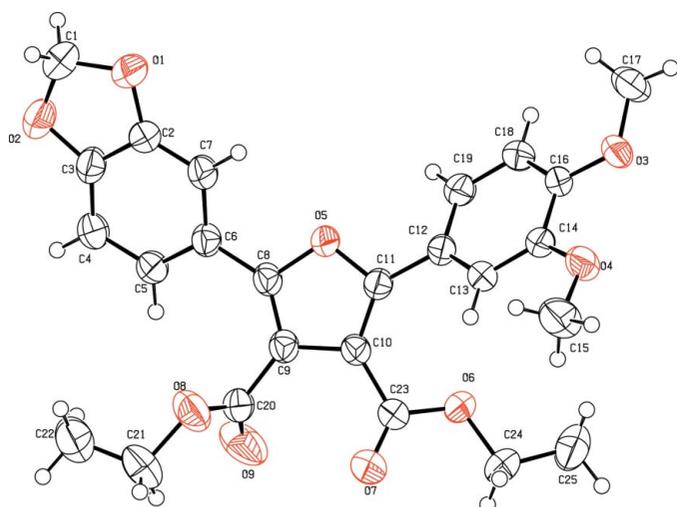


Figure 1
View of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

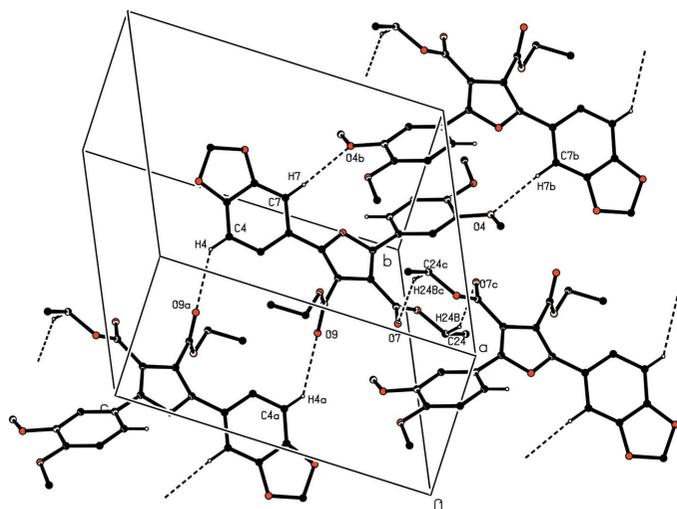


Figure 2
The molecular packing of (I). Dashed lines indicate hydrogen bonds. [Symmetry codes: (a) $-x, 1 - y, 1 - z$; (b) $1 - x, 1 - y, -z$; (c) $1 - x, 2 - y, -z$.]

Crystal data

$C_{25}H_{24}O_9$ $Z = 2$
 $M_r = 468.44$ $D_x = 1.383 \text{ Mg m}^{-3}$
 Triclinic, $P\bar{1}$ Mo $K\alpha$ radiation
 $a = 7.8137(9) \text{ \AA}$ Cell parameters from 2522 reflections
 $b = 11.0275(12) \text{ \AA}$ $\theta = 2.3\text{--}27.2^\circ$
 $c = 13.9703(15) \text{ \AA}$ $\mu = 0.11 \text{ mm}^{-1}$
 $\alpha = 80.796(2)^\circ$ $T = 292(2) \text{ K}$
 $\beta = 75.547(2)^\circ$ Block, colorless
 $\gamma = 76.001(2)^\circ$ $0.30 \times 0.30 \times 0.30 \text{ mm}$
 $V = 1124.7(2) \text{ \AA}^3$

Data collection

Bruker SMART APEX CCD area-detector diffractometer 4348 independent reflections
 ω scans 3217 reflections with $I > 2\sigma(I)$
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $R_{\text{int}} = 0.040$
 $T_{\text{min}} = 0.969, T_{\text{max}} = 0.969$ $\theta_{\text{max}} = 26.0^\circ$
 6449 measured reflections $h = -9 \rightarrow 9$
 $k = -13 \rightarrow 13$
 $l = -11 \rightarrow 17$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.126$
 $S = 0.98$
 4348 reflections
 311 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0709P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

C1—O2	1.420 (3)	C10—C23	1.471 (2)
C1—O1	1.429 (2)	C11—O5	1.3630 (19)
C2—O1	1.368 (2)	C14—O4	1.3629 (19)
C3—C4	1.369 (3)	C16—O3	1.3693 (19)
C6—C8	1.456 (2)	C20—O9	1.189 (2)
C8—C9	1.359 (2)	C20—O8	1.317 (2)
C8—O5	1.3760 (19)	C23—O7	1.1984 (19)
C10—C11	1.370 (2)	C23—O6	1.336 (2)
O2—C1—O1	108.47 (15)	O5—C11—C10	108.69 (13)
O1—C2—C3	109.74 (15)	O5—C11—C12	114.49 (13)
O2—C3—C2	109.97 (16)	C2—O1—C1	105.66 (15)
O5—C8—C6	114.98 (14)	C11—O5—C8	108.91 (12)
C7—C6—C8—C9	156.44 (19)	C10—C9—C20—O9	−64.6 (3)
C5—C6—C8—O5	156.00 (15)	C10—C9—C20—O8	115.77 (18)
C6—C8—C9—C20	2.5 (3)	C11—C10—C23—O7	153.59 (19)
C23—C10—C11—C12	−4.9 (3)	C9—C10—C23—O7	−24.7 (3)
C10—C11—C12—C19	146.03 (19)	C9—C10—C23—O6	155.00 (15)
O5—C11—C12—C13	138.58 (15)	C10—C23—O6—C24	173.62 (15)
C8—C9—C20—O9	111.3 (2)	O9—C20—O8—C21	−1.2 (3)

Table 2

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
C4—H4 \cdots O9 ⁱ	0.93	2.54	3.285 (2)	137
C24—H24B \cdots O7 ⁱⁱ	0.97	2.57	3.445 (3)	151
C7—H7 \cdots O4 ⁱⁱⁱ	0.93	2.43	3.358 (2)	172

Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $-x + 1, -y + 1, -z$; (iii) $-x + 1, -y + 2, -z$.

H atoms were placed in idealized positions and constrained to ride on their parent atoms. Constrained C—H distances: 0.93 \AA for aromatic CH, 0.97 \AA for methylene CH_2 and 0.96 \AA for methyl CH_3 . Fixed isotropic $U_{\text{iso}}(\text{H})$ parameters: $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ for others. Methyl groups were allowed to rotate freely about their C— CH_3 bonds.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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