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Diethyl 2-(1,3-benzodioxol-5-yl)-5-(3,4-dimethoxyphenyl)furan-3,4-dicarboxylate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.126
Data-to-parameter ratio = 14.0

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

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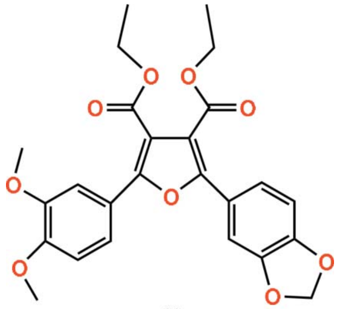
In the title compound, $C_{25}H_{24}O_9$, the substituted benzene rings are twisted away from the furan ring. The dihedral angle between the two benzene rings is 52.1 (1)°. In the crystal structure, the molecules exist as hydrogen-bonded dimers, the molecules being connected through very weak C—H···O 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).



(I)

In compound (I), the furan ring is planar and the two substituted benzene rings are twisted away from it (Fig. 1). The C12/C13/C14/C16/C18/C19 and C2–C7 benzene rings form dihedral angles with the furan ring of 39.5 (2) and 23.4 (1)°, respectively. The dihedral angle between the two benzene rings is 52.1 (1)°. The C2–C7 aromatic ring is effectively coplanar with the five-membered C1/O1/C2/C3/O2 ring, as seen in the dihedral angle between their planes of 1.6 (1)°. 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 C—H···O hydrogen bonds (Table 2). The dimers are interlinked also through very weak C—H···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.

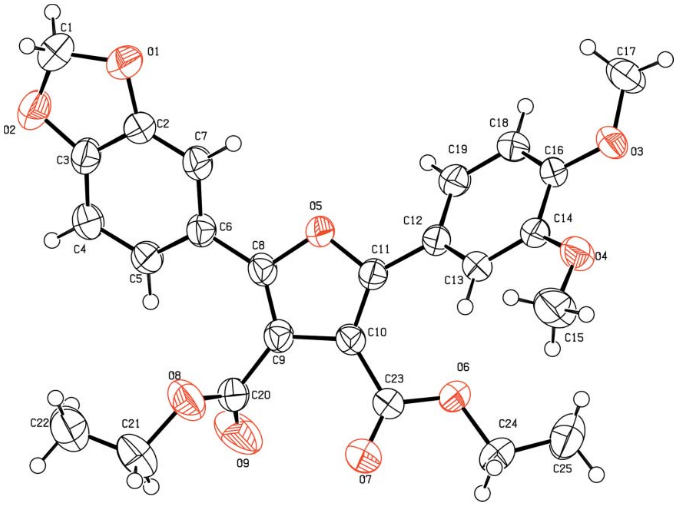


Figure 1
View of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

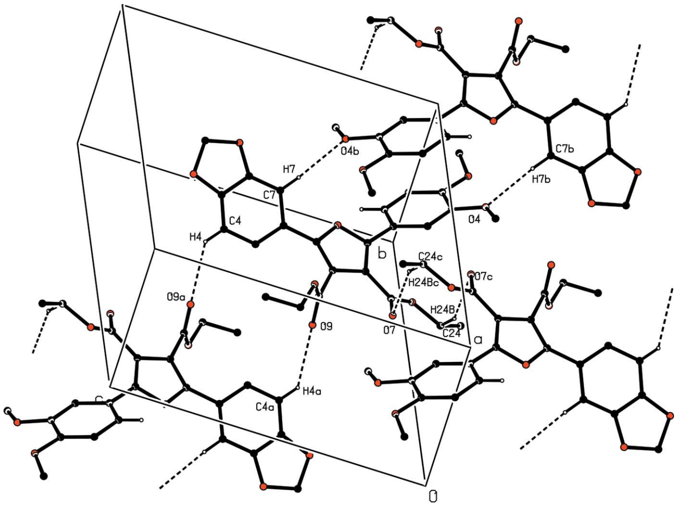


Figure 2
The molecular packing of (I). Dashed lines indicate hydrogen bonds. [Symmetry codes: (*a*) $-x, 1-y, 1-z$; (*b*) $1-x, 1-y, -z$; (*c*) $1-x, 2-y, -z$.]

Crystal data

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

Data collection

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

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

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 (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O9$^{\rm i}$	0.93	2.54	3.285 (2)	137
C24—H24*B*···O7$^{\rm ii}$	0.97	2.57	3.445 (3)	151
C7—H7···O4$^{\rm iii}$	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 Å for aromatic CH, 0.97 Å for methylene CH_2 and 0.96 Å for methyl CH_3. Fixed isotropic $U_{\rm iso}$(H) parameters: $1.5U_{\rm eq}$(C) for methyl H atoms and $1.2U_{\rm eq}$(C) for others. Methyl groups were allowed to rotate freely about their C—CH_3 bonds.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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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