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2,5-Bis(2-methoxyphenyl)furan

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.139
Data-to-parameter ratio = 16.2

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

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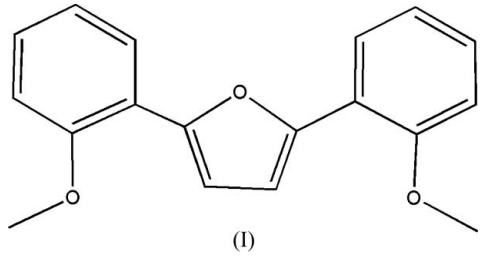
In the title compound, $C_{18}H_{16}O_3$, the dihedral angles between the two benzene rings and the furan ring are 3.7 (1) and 1.0 (1)°. C—H···π and π–π interactions are observed in the crystal structure.

Comment

We have synthesized 2,5-bis(2-methoxyphenyl)furan, (I), according to the literature method of Wu *et al.* (1997) and its structure is reported here.



(I)

The molecule is essentially planar (Fig. 1). Selected bond lengths and angles are listed in Table 1. C—H···π and π–π interactions are observed in the crystal structure (see Table 2 and Fig. 2). Analysis using *PLATON* (Spek, 2003) shows that the distance between the centroids of the C2–C7 and C12^{i}–C17^{i} benzene rings is 3.89 (1) Å [symmetry code: (i) *x*, 1 + *y*, *z*].

Experimental

3-Ethoxy-1-(2-methoxyphenyl)propan-1-one was first synthesized according to the literature (Pelter *et al.*, 1982). Sodium hydride (0.4 g, 80%) was washed with dry pentane and then suspended in dry CH_2Cl_2 (10 ml). To this was added a solution of ethyl 3-(2-methoxyphenyl)-3-oxopropanoate (2.2 g, 10 mmol) in dry CH_2Cl_2 (15 ml) and then a solution of ethyl 2-bromo-3-(2-methoxyphenyl)-3-oxopropanoate (3 g, 10 mmol) in dry CH_2Cl_2 was added. The product was then refluxed with stirring for 3 h. The suspension was cooled, washed with water (20 ml), and dried (Na_2SO_4). After removal of the solvent, the residue was purified, affording diethyl 2,3-bis(2-methoxybenzoyl)succinate. Toluene-*p*-sulfonic acid (5 g) was added to a solution of diethyl 2,3-bis(2-methoxybenzoyl)succinate (2.2 g, 5 mmol) in dry benzene (50 ml). The mixture was refluxed for 8 h and concentrated. The residue was chromatographed on silica gel (light petroleum–ethyl acetate, 8:1 (*v*/*v*) to give diethyl 2,5-bis(2-methoxyphenyl)furan-3,4-dicarboxylate which was hydrogenated, oxidized and decarboxylated to give the title compound. Crystals suitable for X-ray analysis were obtained by recrystallization of the the title compound from ethanol over a period of two weeks.

Crystal data

$C_{18}H_{16}O_3$
M_r = 280.31
Monoclinic, $P2/c$
a = 15.4110 (18) Å
b = 6.6402 (8) Å
c = 14.6523 (17) Å
β = 108.898 (2)°
V = 1418.6 (3) Å^3
Z = 4
D_x = 1.312 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1227 reflections
θ = 2.8–23.2°
μ = 0.09 mm^{-1}
T = 292 (2) K
Block, yellow
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.976, T_{max} = 0.984
8057 measured reflections
3106 independent reflections
1899 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 27.0°
$h = -19 \rightarrow 19$
$k = -8 \rightarrow 8$
$l = -14 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.139
S = 1.03
3106 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.0627P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.423 (2)	C11—O3	1.376 (2)
C2—O1	1.369 (2)	C12—C13	1.392 (2)
C2—C7	1.407 (3)	C12—C17	1.402 (2)
C6—C7	1.387 (2)	C17—O2	1.378 (2)
C7—C8	1.460 (2)	C18—O2	1.422 (2)
C2—C7—C8	122.10 (18)	O3—C11—C12	114.86 (15)
C9—C8—C7	136.74 (18)	O2—C17—C12	115.51 (16)
O3—C8—C7	114.63 (16)	C2—O1—C1	117.61 (16)
C10—C11—C12	136.69 (17)	C8—O3—C11	107.83 (14)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of rings C12–C17, C2–C7 and O3/C8–C11, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···*Cg*1^{i}	0.93	2.80	3.541 (1)	137
C16—H16···*Cg*2^{ii}	0.93	2.95	3.722 (1)	142
C18—H18*A*···*Cg*3^{iii}	0.96	3.24	4.091 (1)	149

Symmetry codes: (i) $x, -y+1, z-\frac{3}{2}$; (ii) $x, -y, z-\frac{1}{2}$; (iii) $x, y-1, z$.

All H atoms were placed at 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_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and U_{iso}(H) = 1.2U_{eq}(C) for all other 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: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

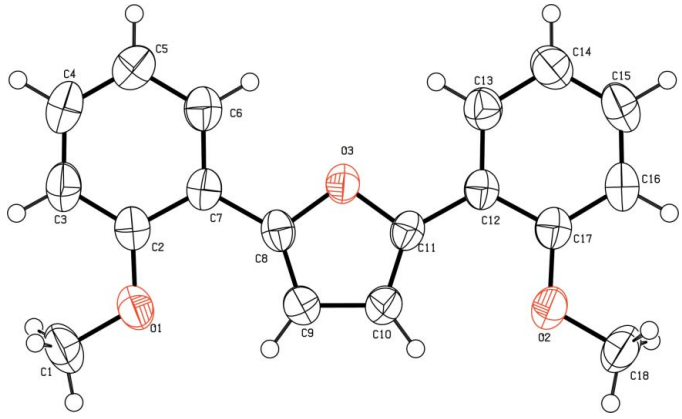


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids.

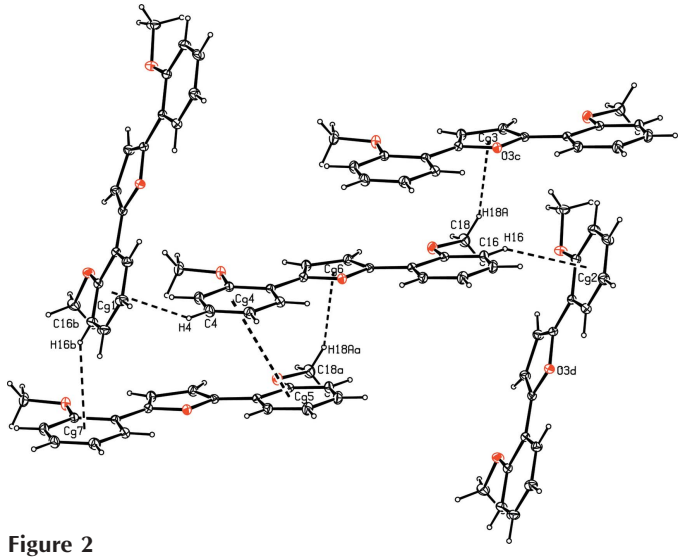


Figure 2
A crystal packing diagram of (I), showing the C—H–π and π–π interactions as dashed lines. [Symmetry codes: (*a*) $x, 1+y, z$; (*b*) $x, 1-y, -\frac{1}{2}+z$; (*c*) $x, -y, \frac{1}{2}+z$; (*d*) $x, -1+y, z$.]

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