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(*E*)-1,3-Di(2-furyl)-2-propen-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.095
Data-to-parameter ratio = 12.4

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

The structure of the title compound, $C_{11}H_8O_3$, contains two crystallographically independent molecules in the asymmetric unit, both of them located in general positions. Both molecules are non-planar; the dihedral angles between the furyl rings are 10.43 (6) and 11.59 (7)°. The crystal structure is stabilized by weak intra- and intermolecular C—H···O and C—H···π interactions.

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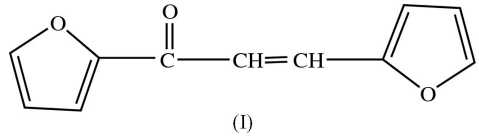
Comment

The title compound, (I), $C_{11}H_8O_3$, is a derivative of chalcone, which is 1,3-diphenyl-2-propen-1-one. Depending on the substitution pattern of the two aromatic rings, a wide range of pharmacological activities have been identified for various chalcones. Chalcones show an impressive array of pharmacological activities, such as antiprotozoal (Nielsen *et al.*, 1998; Li *et al.*, 1995; Liu *et al.*, 2001), anti-inflammatory (Hsieh *et al.*, 1998), nitric oxide inhibition (Rojas *et al.*, 2002) or anticancer properties.



(I)

The crystal structure contains two crystallographically independent molecules in the asymmetric unit, both of them located in general positions. The furyl rings in both molecules are twisted, and the dihedral angles between the furyl rings are 10.43 (6) and 11.59 (7)° (Fig. 1). The geometric parameters of the furyl rings are in the normal ranges and are comparable to those observed in the related compound 2-cyano-*N*-furfuryl-3-(2-furyl)acrylamide (Pomés Hernandez *et al.*, 1996).

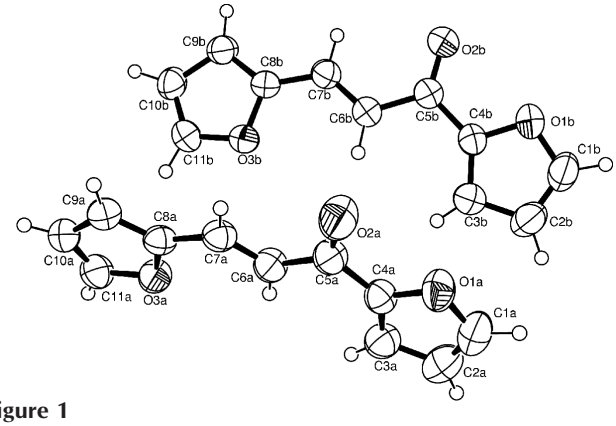


Figure 1
The asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level and the atom-numbering scheme.

In the crystal structure of (I), molecules are connected *via* weak C—H···O interactions into chains that extend in the direction of the *b* axis (Fig. 2 and Table 2). There are additional short contacts between the H atoms and the centroids of the furyl rings (C11*a*—H11*a*···*Cg*4 and C11*b*—H11*b*···*Cg*3; *Cg*4 is the centroid of ring O3*b*—C11*b* and *Cg*3 is the centroid of ring O3*a*—C11*a*), indicating weak C—H···π interactions (Table 2).

Experimental

2-Acetylfuran (0.01 mol) and 2-furaldehyde (0.01 mol) were dissolved in ethanol (25 ml) and the solution was stirred in an ice-bath. Sodium hydroxide (0.5 g, 0.0125 mol) dissolved in water (2.5 ml) was added dropwise to the cooled solution, keeping the temperature below 303 K during this mixing process. The solution was stirred for 3 h at 288–303 K. The resulting precipitate was filtered off, and washed with water and ethanol. After drying, (I) was recrystallized from methanol.

Crystal data

$C_{11}H_8O_3$
M_r = 188.17
Monoclinic, $P2_1/c$
a = 15.1420 (10) Å
b = 11.6395 (8) Å
c = 11.2429 (14) Å
β = 111.363 (7)°
V = 1845.4 (3) Å^3
Z = 8
D_x = 1.355 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 34 010 reflections
θ = 1.4–27.3°
μ = 0.10 mm^{-1}
T = 293 (2) K
Prism, yellow
0.56 × 0.46 × 0.32 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: none
35 020 measured reflections
3920 independent reflections
3179 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 26.8°
$h = -19 \rightarrow 19$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.095
S = 1.03
3920 reflections
317 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.2469P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1*a*—C2*a*	1.329 (3)	C5*b*—O2*b*	1.2216 (15)
C1*a*—O1*a*	1.356 (2)	C8*a*—C9*a*	1.3458 (19)
C1*b*—C2*b*	1.321 (2)	C8*a*—O3*a*	1.3766 (15)
C1*b*—O1*b*	1.3575 (18)	C8*b*—C9*b*	1.3523 (18)
C2*a*—C3*a*	1.409 (2)	C8*b*—O3*b*	1.3721 (14)
C2*b*—C3*b*	1.413 (2)	C9*a*—C10*a*	1.413 (2)
C3*a*—C4*a*	1.348 (2)	C9*b*—C10*b*	1.4099 (19)
C3*b*—C4*b*	1.3456 (18)	C10*a*—C11*a*	1.327 (2)
C4*a*—O1*a*	1.3641 (16)	C10*b*—C11*b*	1.329 (2)
C4*b*—O1*b*	1.3642 (15)	C11*a*—O3*a*	1.3651 (16)
C5*a*—O2*a*	1.2261 (16)	C11*b*—O3*b*	1.3640 (16)
C4*a*—C5*a*—C6*a*	116.46 (12)	C6*a*—C7*a*—C8*a*	127.21 (12)
C4*b*—C5*b*—C6*b*	116.82 (11)	C6*b*—C7*b*—C8*b*	127.90 (12)

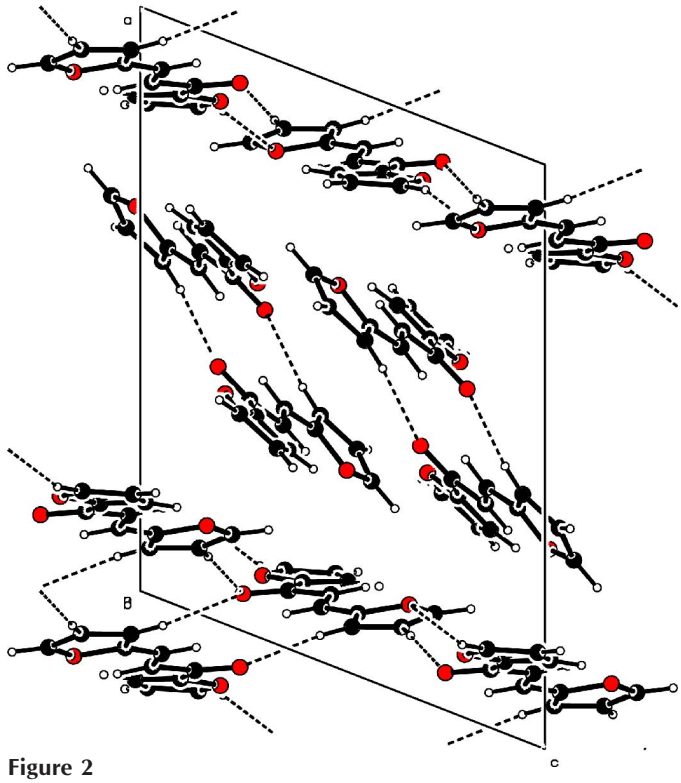


Figure 2
The crystal structure of (I), showing the linkage of molecules *via* C—H···O hydrogen bonding (hydrogen bonds are shown as dashed lines).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1*b*—H1*b*···O3*b*^{i}	0.96 (2)	2.56 (2)	3.4812 (19)	162 (2)
C9*a*—H9*a*···O2*a*^{ii}	0.97 (2)	2.47 (2)	3.4402 (18)	174 (1)
C9*b*—H9*b*···O2*b*^{iii}	0.96 (2)	2.51 (2)	3.4596 (17)	174 (1)
C10*b*—H10*b*···O2*b*^{iv}	0.97 (2)	2.53 (2)	3.4786 (17)	168 (1)
C11*a*—H11*a*···*Cg*4^{v}	0.94 (2)	2.84 (2)	3.5765 (19)	137 (1)
C11*b*—H11*b*···*Cg*3^{vi}	0.95 (2)	2.84 (2)	3.6160 (17)	140 (1)

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $x, y-1, z$; (vi) $x, -y-\frac{1}{2}, z-\frac{1}{2}$. *Cg*4 and *Cg*3 are the centroids of rings O3*b*–C11*b* and O3*a*–C11*a*, respectively.

All H atoms were found in a difference electron-density map and were refined with isotropic displacement parameters. C—H distances are in the range 0.896 (16)–0.99 (2) Å.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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