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(*E*)-4-(4-Ethoxyphenyl)but-3-en-2-one

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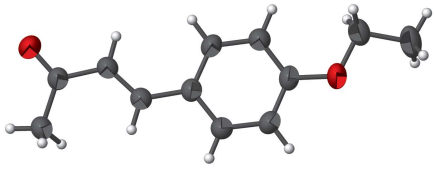
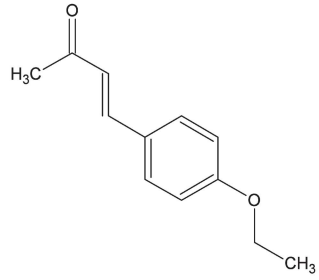
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{12}H_{14}O_2$, the benzene ring makes dihedral angles of 5.03 (8) and 5.37 (15)° with the mean planes of the but-3-en-2-one group and the ethoxy group, respectively. In the crystal, molecules are linked by two pairs of C—H···O hydrogen bonds forming inversion dimers, which enclose an $R_2^2(8)$ ring motif flanked by two $R_2^1(7)$ loops.

3D view



Chemical scheme



Structure description

Chalcones belonging to the flavonoid family constitute an important group of natural products due to their unforeseen pharmacological potential. Chemically they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β-unsaturated carbonyl system. Chalcones have been reported to possess numerous biological activities such as antimicrobial, anti-inflammatory, antimalarial, anti-leishmanial, antioxidant and antitubercular activities (Lin *et al.*, 2002; Sivakumar *et al.*, 2007). The reactive α,β-unsaturated keto group in chalcone derivatives was observed to be responsible for their antimicrobial activity.

In the title compound, Fig. 1, both the but-3-en-2-one group and the ethoxy group are −antiperiplanar (−*ap*) with respect to the benzene ring, as indicated by the torsion angles C7—C6—C9—C10 = −179.84 (14)° and C7—C8—C3—O1 = −178.41 (13)°. The but-3-en-2-one group and the ethoxy group make dihedral angles of 5.03 (8) and 5.37 (15)°, respectively, with the benzene ring.

In the crystal, molecules are linked by two pairs of C—H···O hydrogen bonds forming inversion dimers, which enclose an $R_2^2(8)$ ring motif flanked by two $R_2^1(7)$ loops (Table 1 and Fig. 2).

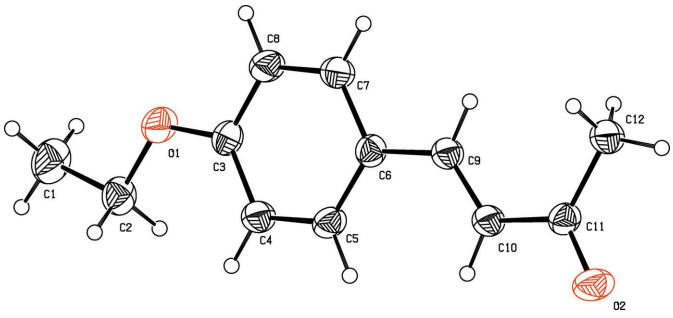


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

Synthesis and crystallization

In a 250 ml round-bottom flask acetone (0.5 mmol) and 4-ethoxybenzaldehyde (0.5 mmol) were taken and 120 ml of absolute alcohol was added. The mixture was stirred at room temperature for 5 min, then 10% sodium hydroxide solution was added and the mixture was stirred for 2 h. The yellow-coloured precipitate generated by adding a sufficient amount of ice-cold water was filtered, washed with distilled water and then dried. The crude product was recrystallized twice from absolute alcohol yielding colourless block-like crystals (yield 78%).

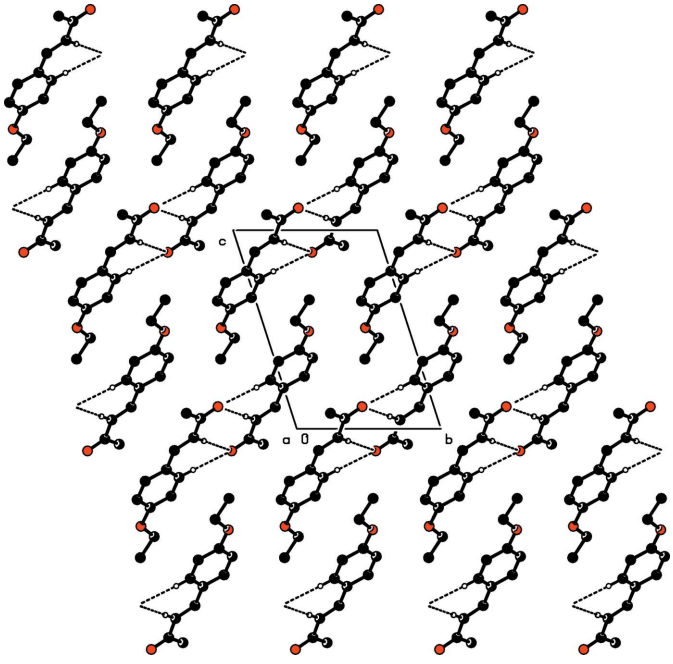


Figure 2
The crystal packing of the title compound, viewed along the *a* axis. The C—H···O hydrogen bonds are shown as dashed lines (see Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2^{i}	0.93	2.50	3.4298 (17)	178
C10—H10···O2^{i}	0.93	2.57	3.5006 (17)	179

Symmetry code: (i) $-x, -y-1, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{14}O_2$
M_r	190.23
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	5.7634 (2), 8.2218 (2), 12.0915 (3)
α, β, γ (°)	105.5413 (14), 102.5395 (16), 97.4291 (14)
V (Å^3)	528.03 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.25 × 0.25
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.976, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7360, 1858, 1589
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.121, 1.03
No. of reflections	1842
No. of parameters	130
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.13

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *ORTEP-3 for Windows* (Farrugia, 2012).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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(*E*)-4-(4-Ethoxyphenyl)but-3-en-2-one

Crystal data

$C_{12}H_{14}O_2$
M_r = 190.23
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 5.7634 (2) Å
b = 8.2218 (2) Å
c = 12.0915 (3) Å
α = 105.5413 (14)°
β = 102.5395 (16)°
γ = 97.4291 (14)°
V = 528.03 (3) Å^3
Z = 2
$F(000)$ = 204
D_x = 1.196 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1858 reflections
θ = 1.8–25.0°
μ = 0.08 mm^{-1}
T = 296 K
Block, colorless
0.30 × 0.25 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.976, T_{max} = 0.980
7360 measured reflections
1858 independent reflections
1589 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −6→6
k = −9→9
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.121
S = 1.03
1842 reflections
130 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.0923P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.029 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.0703 (4)	0.3733 (2)	0.64921 (17)	0.0787 (6)
H1A	1.1266	0.4691	0.6242	0.118*
H1B	1.2069	0.3329	0.6860	0.118*
H1C	0.9777	0.4089	0.7053	0.118*
C2	0.9134 (3)	0.2306 (2)	0.54296 (13)	0.0568 (4)
H2A	1.0055	0.1920	0.4860	0.068*
H2B	0.8529	0.1336	0.5671	0.068*
C3	0.5377 (3)	0.19381 (18)	0.39674 (12)	0.0474 (4)
C4	0.5370 (3)	0.02313 (18)	0.33933 (13)	0.0504 (4)
H4	0.6675	−0.0263	0.3639	0.060*
C5	0.3417 (3)	−0.07347 (17)	0.24538 (12)	0.0485 (4)
H5	0.3427	−0.1878	0.2076	0.058*
C6	0.1442 (2)	−0.00352 (17)	0.20622 (11)	0.0439 (3)
C7	0.1524 (3)	0.16901 (19)	0.26405 (13)	0.0526 (4)
H7	0.0239	0.2197	0.2389	0.063*
C8	0.3449 (3)	0.26628 (19)	0.35711 (13)	0.0552 (4)
H8	0.3457	0.3814	0.3937	0.066*
C9	−0.0692 (2)	−0.10142 (18)	0.10940 (12)	0.0458 (4)
H9	−0.1907	−0.0412	0.0912	0.055*
C10	−0.1105 (2)	−0.26480 (17)	0.04465 (12)	0.0476 (4)
H10	0.0082	−0.3277	0.0617	0.057*
C11	−0.3285 (3)	−0.35470 (17)	−0.05185 (12)	0.0468 (4)
C12	−0.5374 (3)	−0.26762 (19)	−0.07783 (14)	0.0553 (4)
H12A	−0.4946	−0.1819	−0.1143	0.083*
H12B	−0.5756	−0.2137	−0.0050	0.083*
H12C	−0.6759	−0.3514	−0.1308	0.083*
O1	0.71689 (19)	0.29938 (13)	0.49135 (9)	0.0613 (3)
O2	−0.3390 (2)	−0.50178 (14)	−0.11143 (10)	0.0720 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0714 (12)	0.0707 (12)	0.0673 (11)	−0.0023 (9)	−0.0184 (9)	0.0142 (9)
C2	0.0512 (9)	0.0588 (9)	0.0510 (8)	0.0044 (7)	0.0005 (7)	0.0147 (7)
C3	0.0465 (8)	0.0436 (8)	0.0425 (7)	0.0015 (6)	0.0051 (6)	0.0061 (6)
C4	0.0476 (8)	0.0454 (8)	0.0509 (8)	0.0119 (6)	0.0038 (6)	0.0090 (6)

C5	0.0524 (8)	0.0375 (7)	0.0469 (7)	0.0077 (6)	0.0066 (6)	0.0043 (6)
C6	0.0429 (7)	0.0427 (7)	0.0415 (7)	0.0052 (6)	0.0082 (6)	0.0089 (6)
C7	0.0472 (8)	0.0467 (8)	0.0545 (8)	0.0132 (6)	0.0038 (6)	0.0058 (6)
C8	0.0546 (9)	0.0416 (8)	0.0556 (8)	0.0102 (7)	0.0038 (7)	0.0005 (6)
C9	0.0427 (7)	0.0443 (8)	0.0462 (7)	0.0100 (6)	0.0064 (6)	0.0107 (6)
C10	0.0431 (8)	0.0443 (8)	0.0492 (8)	0.0109 (6)	0.0032 (6)	0.0104 (6)
C11	0.0471 (8)	0.0408 (8)	0.0455 (7)	0.0069 (6)	0.0040 (6)	0.0093 (6)
C12	0.0475 (8)	0.0515 (9)	0.0555 (8)	0.0108 (7)	0.0000 (6)	0.0080 (7)
O1	0.0563 (7)	0.0474 (6)	0.0569 (6)	0.0046 (5)	−0.0103 (5)	0.0007 (5)
O2	0.0704 (8)	0.0453 (6)	0.0747 (8)	0.0177 (5)	−0.0096 (6)	−0.0035 (5)

Geometric parameters (Å, º)

C1—C2	1.502 (2)	C6—C7	1.393 (2)
C1—H1A	0.9600	C6—C9	1.4648 (19)
C1—H1B	0.9600	C7—C8	1.372 (2)
C1—H1C	0.9600	C7—H7	0.9300
C2—O1	1.4281 (18)	C8—H8	0.9300
C2—H2A	0.9700	C9—C10	1.322 (2)
C2—H2B	0.9700	C9—H9	0.9300
C3—O1	1.3608 (17)	C10—C11	1.4653 (19)
C3—C8	1.383 (2)	C10—H10	0.9300
C3—C4	1.388 (2)	C11—O2	1.2166 (17)
C4—C5	1.385 (2)	C11—C12	1.4966 (19)
C4—H4	0.9300	C12—H12A	0.9600
C5—C6	1.3897 (19)	C12—H12B	0.9600
C5—H5	0.9300	C12—H12C	0.9600
C2—C1—H1A	109.5	C7—C6—C9	119.14 (13)
C2—C1—H1B	109.5	C8—C7—C6	121.84 (14)
H1A—C1—H1B	109.5	C8—C7—H7	119.1
C2—C1—H1C	109.5	C6—C7—H7	119.1
H1A—C1—H1C	109.5	C7—C8—C3	120.25 (13)
H1B—C1—H1C	109.5	C7—C8—H8	119.9
O1—C2—C1	106.73 (13)	C3—C8—H8	119.9
O1—C2—H2A	110.4	C10—C9—C6	128.01 (13)
C1—C2—H2A	110.4	C10—C9—H9	116.0
O1—C2—H2B	110.4	C6—C9—H9	116.0
C1—C2—H2B	110.4	C9—C10—C11	125.16 (13)
H2A—C2—H2B	108.6	C9—C10—H10	117.4
O1—C3—C8	115.88 (13)	C11—C10—H10	117.4
O1—C3—C4	124.88 (13)	O2—C11—C10	119.43 (13)
C8—C3—C4	119.25 (13)	O2—C11—C12	119.80 (13)
C5—C4—C3	119.86 (13)	C10—C11—C12	120.77 (12)
C5—C4—H4	120.1	C11—C12—H12A	109.5
C3—C4—H4	120.1	C11—C12—H12B	109.5
C4—C5—C6	121.55 (13)	H12A—C12—H12B	109.5
C4—C5—H5	119.2	C11—C12—H12C	109.5

C6—C5—H5	119.2	H12A—C12—H12C	109.5
C5—C6—C7	117.24 (13)	H12B—C12—H12C	109.5
C5—C6—C9	123.62 (13)	C3—O1—C2	119.21 (12)
O1—C3—C4—C5	178.51 (13)	C4—C3—C8—C7	1.7 (2)
C8—C3—C4—C5	−1.6 (2)	C5—C6—C9—C10	−0.4 (2)
C3—C4—C5—C6	0.2 (2)	C7—C6—C9—C10	−179.84 (14)
C4—C5—C6—C7	1.1 (2)	C6—C9—C10—C11	−179.57 (12)
C4—C5—C6—C9	−178.37 (12)	C9—C10—C11—O2	174.48 (14)
C5—C6—C7—C8	−1.0 (2)	C9—C10—C11—C12	−5.5 (2)
C9—C6—C7—C8	178.49 (13)	C8—C3—O1—C2	175.46 (13)
C6—C7—C8—C3	−0.4 (2)	C4—C3—O1—C2	−4.6 (2)
O1—C3—C8—C7	−178.41 (13)	C1—C2—O1—C3	−176.21 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.93	2.50	3.4298 (17)	178
C10—H10···O2^{i}	0.93	2.57	3.5006 (17)	179

Symmetry code: (i) −*x*, −*y*−1, −*z*.