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(*E*)-3-(2,5-Difluorophenyl)-1-phenylprop-2-en-1-one

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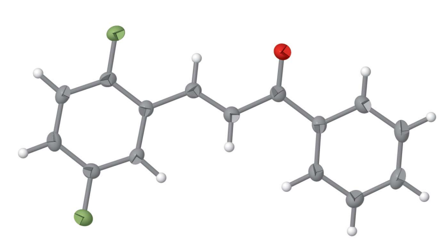
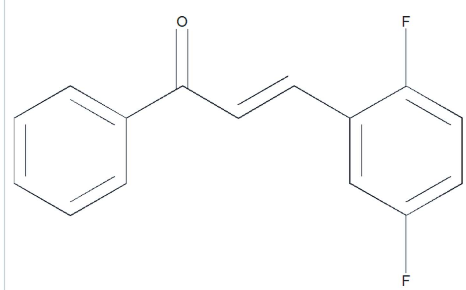
Structural data: full structural data are available from iucrdata.iucr.org

The title chalcone derivative, $C_{15}H_{10}F_2O$, is almost planar, with the benzene ring being inclined to the phenyl ring by 7.45 (9)°. The conformation about the C═C bond is *E*. In the crystal, molecules are linked by two pairs of C—H···F hydrogen bonds, forming inversion dimers enclosing $R_2^2(8)$ and $R_2^1(10)$ ring motifs. The dimers stack along the *a* axis with the separation of the C═C bonds being 4.2926 (4) Å.

3D view



Chemical scheme



Structure description

Chalcone is a generic term given to compounds having the 1,3-diphenylprop-2-en-1-one moiety. They were the first isolatable compounds from flavonoid biosynthesis in plants (Bohm, 1998; Yazdan *et al.*, 2015) and are widely distributed in fruits, vegetables, spices, tea and soy-based foodstuffs. They have interesting pharmacological properties (Di Carlos *et al.*, 1999; Das & Manna, 2016), including analgesic, antioxidant, antifungal, antibacterial, antiprotozoal, gastric 'protectant', antimutagenic, antitumorogenic, anti-inflammatory (Yadav *et al.*, 2011) and antineurodegeneration properties (Sahu *et al.*, 2012; Singh *et al.*, 2014). The title chalcone derivative was obtained by a Claisen–Schimdt condensation in a basic solution of ethanol and water between 2,5-difluorobenzaldehyde and acetophenone.

The molecular structure of the title compound is illustrated in Fig. 1. The structure is almost planar, with the dihedral angle between the benzene (C1–C6) and phenyl (C10–

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C1—H1$\cdots$F1^{i}	0.95	2.49	3.440 (2)	174
C11—H11$\cdots$F1^{i}	0.95	2.46	3.379 (2)	163

Symmetry code: (i) $-x+2, -y+1, -z+1$.

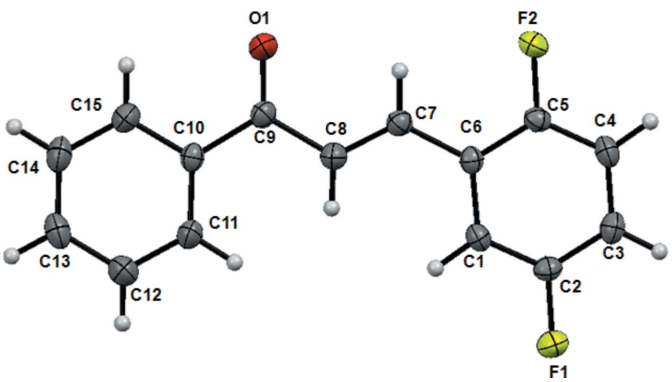


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

C15) rings being 7.45 (9)°. The conformation of the keto group (C9=O1) with respect to the olefinic double bond (C7=C8) is *cis*. The conformation about the C7=C8 bond itself is *E*, with the 2,5-difluorobenzene ring opposite to the phenyl ring.

In the crystal, molecules are linked by two pairs of C—H$\cdots$F hydrogen bonds, forming inversion dimers enclosing $R_2^2(8)$ and $R_2^1(10)$ rings (Table 1 and Fig. 2). The separation distances of bonds C7=C8$\cdots$C7^{i}=C8^{i} [symmetry code: (i) $1+x, y, z$] of adjacent molecules stacked along the *a* axis is 4.2926 (4) Å, with an angle of 52.0 (1)° (Fig. 3). This distance is in the range for relevant distances enrolled in photochemical [2 + 2] cycloaddition reactions between olefins (Sonoda, 2011).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}F_2O$
M_r	244.23
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	4.2926 (4), 17.7983 (13), 14.8522 (13)
β (°)	94.757 (4)
V (Å^3)	1130.81 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.31 × 0.23 × 0.16
Data collection	
Diffractometer	Bruker D8 Venture
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5621, 2322, 1740
R_{int}	0.052
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.136, 1.07
No. of reflections	2322
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.24

Computer programs: *SAINT* and *APEX3* (Bruker, 2015), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

Synthesis and crystallization

Potassium hydroxide in 10% molar (0.0026 g ml^{-1}) concentration relative to the ketone was added to an ethanol–water (6:1) mixture. To this solution, the total amount of 2,5-difluorobenzaldehyde (582 mg, 4.1 mmol) and half of the acetophenone (288 mg, 2.4 mmol) were added at room temperature. After approximately 1–2 h, the reminder of the acetophenone was added under constant stirring at 298 K, and

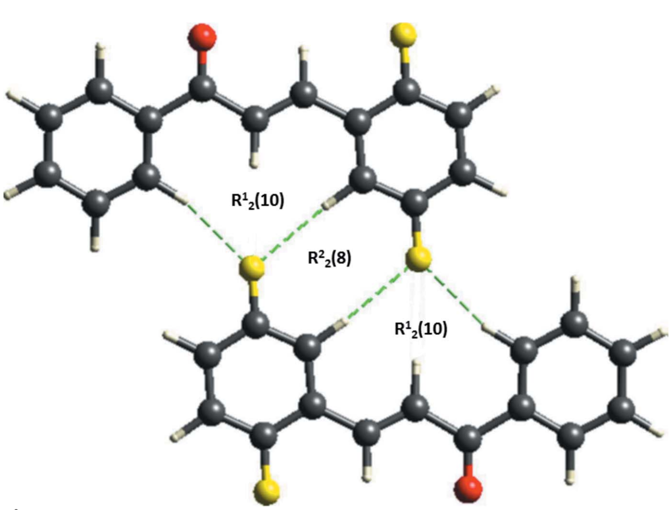


Figure 2
A view of the inversion dimers formed by two pairs of C—H$\cdots$F hydrogen bonds (see Table 1).

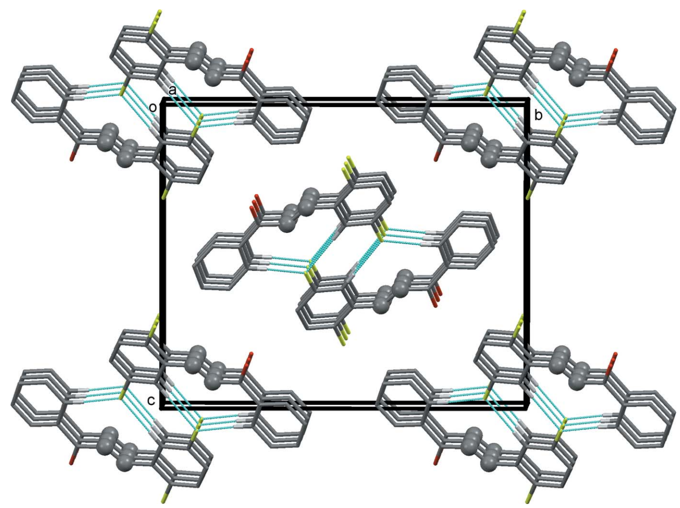


Figure 3
A view along the *a* axis of the crystal packing of the title compound. The C—H$\cdots$F hydrogen bonds are shown as dashed lines (see Table 1) and the olefin C atoms (C7 and C8) as grey balls.

the reaction was continued until the appearance of a yellow precipitate. The reaction mixture was filtered and the solid residue obtained was washed with cold water until a neutral pH was attained and was then recrystallized a number of times from a mixture of ethanol and water (yield 65%, m.p. 361–363 K). Yellow single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution of the title compound (m.p. 363 K). Spectroscopic data: IR (KBr) ν (cm^{-1}): 1674.3 (C═O *s-cis*); 1655.0 (C═O *s-trans*); 1610.9 (C═C *s-cis*). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90–6.50 (*m*, 8H, aromatic); 7.83 (*d*, H_7); 7.59 (*d*, H_8). ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.8 (C═O); 160.5 (*dd*, C_2); 155.0 (*dd*, C_5); 137.6 (C_{10}); 135.9 (C_7); 133.0 (C_{13}); 128.6 (C_{14}═C_{12}); 128.5 (C_{15}═C_{11}); 125.3 (C_8); 118.5 (*d*, C_3); 117.9 (*d*, C_4); 117.2 (*d*, C_1). (MS *m*/*z* (%): 244 ($M^{+\cdot}$, 100); 243 (29); 225 (36); 215 (18); 214 (5); 201 (7); 196 (11); 195 (6); 167 (42); 139 (29); 119 (36); 105 (67); 77 (82).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161295 [doi:10.1107/S2414314616012955]

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Crystal data

$C_{15}H_{10}F_2O$
M_r = 244.23
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 4.2926 (4) Å
b = 17.7983 (13) Å
c = 14.8522 (13) Å
β = 94.757 (4)°
V = 1130.81 (17) Å^3
Z = 4
$F(000)$ = 504
D_x = 1.435 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3798 reflections
θ = 2.7–26.4°
μ = 0.11 mm^{-1}
T = 150 K
Orthombic, colorless
0.31 × 0.23 × 0.16 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: Microfocus sealed tube, Incoatec Iμs
Quazar multilayer mirror monochromator
φ and ω scans
5621 measured reflections
2322 independent reflections
1740 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 26.4°, θ_{min} = 2.3°
$h = -5 \rightarrow 5$
$k = -21 \rightarrow 22$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.07
2322 reflections
163 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.290P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
F2	0.0822 (3)	0.50588 (6)	0.19482 (7)	0.0330 (3)
F1	0.9771 (3)	0.60432 (6)	0.44588 (7)	0.0351 (3)
O1	0.0788 (4)	0.25342 (7)	0.32124 (9)	0.0367 (4)
C1	0.6528 (4)	0.50652 (10)	0.38831 (11)	0.0229 (4)
H1	0.739	0.4748	0.4354	0.027*
C5	0.3075 (4)	0.52985 (10)	0.25802 (11)	0.0234 (4)
C6	0.4238 (4)	0.47913 (10)	0.32404 (11)	0.0215 (4)
C10	0.3791 (4)	0.21865 (10)	0.45575 (11)	0.0230 (4)
C2	0.7518 (4)	0.57955 (10)	0.38272 (12)	0.0244 (4)
C9	0.2765 (5)	0.27205 (10)	0.38094 (12)	0.0254 (4)
C3	0.6369 (5)	0.62892 (10)	0.31648 (12)	0.0267 (4)
H3	0.7128	0.679	0.3146	0.032*
C7	0.3066 (4)	0.40188 (10)	0.32591 (11)	0.0241 (4)
H7	0.1368	0.3892	0.2835	0.029*
C4	0.4083 (4)	0.60333 (10)	0.25306 (12)	0.0269 (4)
H4	0.3216	0.6357	0.2067	0.032*
C8	0.4166 (5)	0.34818 (10)	0.38147 (12)	0.0269 (4)
H8	0.5912	0.3588	0.4231	0.032*
C15	0.2643 (5)	0.14540 (11)	0.45084 (13)	0.0309 (5)
H15	0.1283	0.1304	0.4003	0.037*
C13	0.5437 (5)	0.11552 (11)	0.59271 (13)	0.0330 (5)
H13	0.601	0.0802	0.6392	0.04*
C11	0.5791 (5)	0.23899 (11)	0.53030 (12)	0.0300 (5)
H11	0.6629	0.2884	0.5342	0.036*
C14	0.3461 (5)	0.09438 (11)	0.51866 (14)	0.0360 (5)
H14	0.2666	0.0446	0.5145	0.043*
C12	0.6573 (5)	0.18811 (12)	0.59882 (13)	0.0362 (5)
H12	0.7893	0.2031	0.6502	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F2	0.0354 (7)	0.0304 (6)	0.0309 (6)	0.0010 (5)	−0.0107 (5)	0.0019 (4)
F1	0.0362 (7)	0.0324 (6)	0.0351 (6)	−0.0080 (5)	−0.0070 (5)	0.0000 (5)
O1	0.0482 (10)	0.0251 (7)	0.0343 (7)	−0.0044 (7)	−0.0123 (7)	−0.0008 (6)
C1	0.0244 (9)	0.0224 (9)	0.0217 (9)	0.0036 (8)	0.0018 (7)	0.0033 (7)
C5	0.0218 (10)	0.0251 (9)	0.0229 (9)	0.0033 (8)	−0.0006 (7)	−0.0012 (7)
C6	0.0223 (9)	0.0198 (9)	0.0228 (9)	0.0028 (7)	0.0041 (7)	0.0003 (7)
C10	0.0247 (10)	0.0187 (9)	0.0261 (9)	0.0022 (7)	0.0050 (7)	−0.0007 (7)
C2	0.0210 (9)	0.0266 (9)	0.0253 (9)	−0.0011 (7)	0.0005 (7)	−0.0016 (7)
C9	0.0300 (10)	0.0207 (9)	0.0254 (9)	0.0012 (8)	0.0012 (8)	−0.0031 (7)
C3	0.0283 (10)	0.0210 (9)	0.0317 (10)	−0.0009 (8)	0.0079 (8)	0.0024 (7)
C7	0.0259 (10)	0.0229 (9)	0.0233 (9)	0.0013 (8)	0.0006 (7)	−0.0022 (7)
C4	0.0287 (10)	0.0243 (9)	0.0279 (9)	0.0043 (8)	0.0033 (8)	0.0078 (7)
C8	0.0279 (10)	0.0236 (9)	0.0284 (10)	−0.0007 (8)	−0.0022 (8)	0.0009 (7)

C15	0.0334 (11)	0.0238 (10)	0.0346 (10)	−0.0041 (8)	−0.0017 (8)	−0.0011 (8)
C13	0.0355 (12)	0.0285 (10)	0.0356 (11)	0.0057 (9)	0.0055 (9)	0.0113 (8)
C11	0.0387 (12)	0.0205 (9)	0.0304 (10)	−0.0025 (8)	−0.0007 (9)	0.0003 (7)
C14	0.0416 (13)	0.0214 (9)	0.0455 (12)	−0.0014 (9)	0.0059 (10)	0.0050 (8)
C12	0.0438 (13)	0.0325 (11)	0.0310 (10)	−0.0018 (10)	−0.0056 (9)	0.0037 (8)

Geometric parameters (Å, º)

F2—C5	1.359 (2)	C3—H3	0.95
F1—C2	1.364 (2)	C7—C8	1.324 (3)
O1—C9	1.221 (2)	C7—H7	0.95
C1—C2	1.372 (2)	C4—H4	0.95
C1—C6	1.400 (2)	C8—H8	0.95
C1—H1	0.95	C15—C14	1.380 (3)
C5—C4	1.381 (3)	C15—H15	0.95
C5—C6	1.394 (2)	C13—C12	1.381 (3)
C6—C7	1.465 (2)	C13—C14	1.384 (3)
C10—C11	1.391 (3)	C13—H13	0.95
C10—C15	1.394 (3)	C11—C12	1.383 (3)
C10—C9	1.500 (2)	C11—H11	0.95
C2—C3	1.379 (3)	C14—H14	0.95
C9—C8	1.482 (3)	C12—H12	0.95
C3—C4	1.380 (3)		
C2—C1—C6	119.48 (16)	C6—C7—H7	117.1
C2—C1—H1	120.3	C3—C4—C5	118.97 (16)
C6—C1—H1	120.3	C3—C4—H4	120.5
F2—C5—C4	117.93 (15)	C5—C4—H4	120.5
F2—C5—C6	118.38 (16)	C7—C8—C9	122.22 (18)
C4—C5—C6	123.69 (17)	C7—C8—H8	118.9
C5—C6—C1	116.38 (16)	C9—C8—H8	118.9
C5—C6—C7	121.15 (16)	C14—C15—C10	120.66 (18)
C1—C6—C7	122.46 (16)	C14—C15—H15	119.7
C11—C10—C15	118.51 (17)	C10—C15—H15	119.7
C11—C10—C9	123.26 (16)	C12—C13—C14	119.74 (18)
C15—C10—C9	118.23 (16)	C12—C13—H13	120.1
F1—C2—C1	118.05 (16)	C14—C13—H13	120.1
F1—C2—C3	118.42 (16)	C12—C11—C10	120.75 (18)
C1—C2—C3	123.53 (17)	C12—C11—H11	119.6
O1—C9—C8	120.61 (17)	C10—C11—H11	119.6
O1—C9—C10	120.63 (16)	C15—C14—C13	120.22 (18)
C8—C9—C10	118.75 (16)	C15—C14—H14	119.9
C2—C3—C4	117.93 (17)	C13—C14—H14	119.9
C2—C3—H3	121	C13—C12—C11	120.10 (19)
C4—C3—H3	121	C13—C12—H12	120
C8—C7—C6	125.74 (17)	C11—C12—H12	120
C8—C7—H7	117.1		

F2—C5—C6—C1	−179.29 (15)	C1—C6—C7—C8	−6.1 (3)
C4—C5—C6—C1	0.7 (3)	C2—C3—C4—C5	−0.6 (3)
F2—C5—C6—C7	−0.2 (3)	F2—C5—C4—C3	−179.97 (16)
C4—C5—C6—C7	179.81 (16)	C6—C5—C4—C3	0.0 (3)
C2—C1—C6—C5	−0.8 (2)	C6—C7—C8—C9	177.78 (16)
C2—C1—C6—C7	−179.88 (16)	O1—C9—C8—C7	9.3 (3)
C6—C1—C2—F1	−179.43 (15)	C10—C9—C8—C7	−169.86 (17)
C6—C1—C2—C3	0.2 (3)	C11—C10—C15—C14	0.3 (3)
C11—C10—C9—O1	−173.28 (18)	C9—C10—C15—C14	−178.73 (19)
C15—C10—C9—O1	5.7 (3)	C15—C10—C11—C12	−1.3 (3)
C11—C10—C9—C8	5.9 (3)	C9—C10—C11—C12	177.74 (19)
C15—C10—C9—C8	−175.08 (17)	C10—C15—C14—C13	0.1 (3)
F1—C2—C3—C4	−179.81 (16)	C12—C13—C14—C15	0.4 (3)
C1—C2—C3—C4	0.6 (3)	C14—C13—C12—C11	−1.4 (3)
C5—C6—C7—C8	174.89 (18)	C10—C11—C12—C13	1.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···F1^{i}	0.95	2.49	3.440 (2)	174
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Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.