Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*E*)-3-(4-Fluorophenyl)-1-(thien-2-yl)-prop-2-en-1-one

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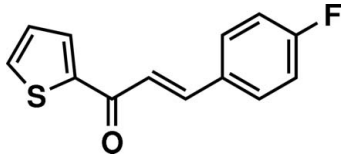
Received 28 October 2007; accepted 31 October 2007

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.051; wR factor = 0.156; data-to-parameter ratio = 25.1.

In the title molecule, $C_{13}H_9FOS$, the dihedral angle between the thiophene ring and the benzene ring is 10.8 (1)°. The crystal packing is stabilized by C—H···O and C—H···π hydrogen bonds.

Related literature

For the uses of chalcones, see Almeida *et al.* (1999); Aries (1972*a*, 1972*b*); Chen *et al.* (1999, 2001); Cole & Julian (1954); Lin *et al.* (2002); Lunardi *et al.* (2003); Main & Old (1977); Tsukiyama *et al.* (2002).



Experimental

Crystal data

$C_{13}H_9FOS$
M_r = 232.27
Monoclinic, $P2_1/n$
a = 12.9010 (4) Å
b = 5.8279 (1) Å
c = 14.5705 (5) Å
β = 94.505 (3)°
V = 1092.11 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 200 (2) K
0.41 × 0.36 × 0.23 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.954, T_{max} = 1.000 (expected range = 0.894–0.937)
15685 measured reflections
3644 independent reflections
2312 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.157
S = 1.02
3644 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1	0.95	2.48	2.822 (2)	101
C16—H16···O1^{i}	0.95	2.59	3.389 (2)	142
C25—H25···F14^{ii}	0.95	2.41	3.153 (2)	135
C13—H13···Cg^{iii}	0.95	2.84	3.567 (2)	134

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $x+1, y-1, z$; (iii) $-x-\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$. Cg is the centroid of the benzene ring.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2543).

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  doi:10.1107/S1600536807054992

supplementary materials

Acta Cryst. (2007). E**63**, o4536 [**doi:10.1107/S1600536807054992**]

(2*E*)-3-(4-Fluorophenyl)-1-(thien-2-yl)prop-2-en-1-one

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Comment

The presence of enone functions in the chalcone molecule confers antibiotic property (Almeida *et al.*, 1999; Cole & Julian, 1954; Main & Old, 1977; and Tsukiyama *et al.*, 2002). This property is enhanced when substitution is made at the α and β positions (Aries, 1972*a*,b). Some substituted chalcones and their derivatives including their heterocyclic analogues are also reported to possess some interesting biological properties. Some of the compounds are claimed to be toxic to animals and insects, and are also reported to possess antileishmanial (Chen *et al.*, 1999, 2001), antitubercular (Lin *et al.*, 2002), trypanocidal (Lunardi *et al.*, 2003) activities.

In the title molecule, $C_{13}H_9FOS$, Fig. 1, the dihedral angle between the thiophene ring and the benzene ring is 10.8 (1)°. The crystal packing is stabilized by C—H···O and C—H..π hydrogen bonds, see Fig. 2 and hydrogen bond table.

Experimental

4-fluorobenzaldehyde (3.32 g, 0.02 mol) in ethanol was mixed with 4-chlorobenzaldehyde (2.54 g, 0.02 mol) in 20 ml e thanol and the mixture was treated with 8 ml of 10% NaOH solution at 283 K and stirred for 8 h. The precipitate obtained was filtered, washed with ethanol and dried. Pale yellow rods of the title compound were grown from a 1:1 (*v*/*v*) solution of acetone and toluene by slow evaporation. The yield of the isolated product was 2.8 g (60%). The colorless prism which was used for data collection was obtained from further recrystallization

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95Å and U_{iso}=1.2 times U_{eq}(C).

Figures

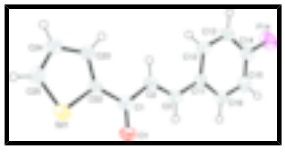

Fig. 1. The molecular structure of the title compound with the atomic numbering and 50% probability displacement ellipsoids. H atoms are shown shown as small spheres of arbitrary radius.

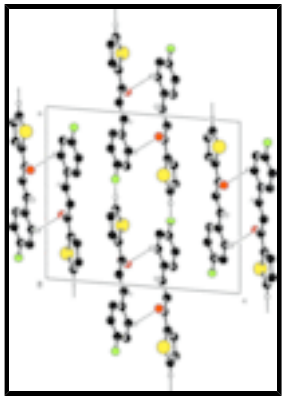

Fig. 2. The molecular packing of the title molecule, viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

(2E)-3-(4-Fluorophenyl)-1-(thien-2-yl)prop-2-en-1-one

Crystal data

$C_{13}H_9FOS$	F_{000} = 480
M_r = 232.27	D_x = 1.413 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 404(1) K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.9010 (4) Å	Cell parameters from 5998 reflections
b = 5.8279 (1) Å	θ = 4.7–32.4º
c = 14.5705 (5) Å	μ = 0.28 mm^{-1}
β = 94.505 (3)º	T = 200 (2) K
V = 1092.11 (5) Å^3	Prism, colorless
Z = 4	0.41 × 0.36 × 0.23 mm

Data collection

Oxford Diffraction Gemini diffractometer	3644 independent reflections
Radiation source: fine-focus sealed tube	2312 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 200(2) K	θ_{max} = 32.5º
φ and ω scans	θ_{min} = 4.7º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	h = −18→18
T_{min} = 0.954, T_{max} = 1.000	k = −8→8
15685 measured reflections	l = −20→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained

$wR(F^2) = 0.157$	$w = 1/[\sigma^2(F_o^2) + (0.0957P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = <0.001$
3644 reflections	$\Delta\rho_{max} = 0.75$ e Å^{-3}
145 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S21	0.34505 (4)	0.05825 (7)	0.39319 (3)	0.0449 (2)
F14	−0.39153 (8)	0.8695 (2)	0.35687 (8)	0.0625 (4)
O1	0.12376 (10)	−0.01134 (19)	0.41781 (10)	0.0530 (4)
C1	0.13970 (12)	0.1849 (3)	0.39121 (11)	0.0364 (4)
C2	0.05678 (12)	0.3568 (3)	0.37578 (11)	0.0366 (5)
C3	−0.03827 (12)	0.3149 (3)	0.40127 (10)	0.0343 (4)
C11	−0.12867 (12)	0.4677 (3)	0.38948 (10)	0.0316 (4)
C12	−0.12682 (12)	0.6792 (3)	0.34484 (11)	0.0375 (5)
C13	−0.21492 (13)	0.8146 (3)	0.33295 (11)	0.0404 (5)
C14	−0.30437 (12)	0.7368 (3)	0.36794 (11)	0.0403 (5)
C15	−0.31018 (13)	0.5316 (3)	0.41429 (11)	0.0414 (5)
C16	−0.22184 (12)	0.3972 (3)	0.42443 (10)	0.0362 (5)
C22	0.24589 (11)	0.2540 (2)	0.37250 (10)	0.0335 (4)
C23	0.28218 (13)	0.4593 (3)	0.34062 (11)	0.0369 (5)
C24	0.39139 (14)	0.4546 (3)	0.33341 (13)	0.0458 (6)
C25	0.43407 (14)	0.2481 (3)	0.35928 (13)	0.0486 (6)
H2	0.07111	0.49883	0.34741	0.0439*
H3	−0.04861	0.17128	0.43003	0.0412*
H12	−0.06388	0.73122	0.32217	0.0450*
H13	−0.21363	0.95721	0.30151	0.0485*
H15	−0.37298	0.48410	0.43852	0.0497*
H16	−0.22420	0.25439	0.45563	0.0435*
H23	0.23933	0.58845	0.32532	0.0443*
H24	0.43017	0.58067	0.31294	0.0549*
H25	0.50601	0.21423	0.35839	0.0583*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S21	0.0424 (3)	0.0302 (2)	0.0620 (3)	0.0089 (2)	0.0029 (2)	0.0011 (2)
F14	0.0470 (6)	0.0594 (7)	0.0808 (8)	0.0278 (6)	0.0026 (6)	0.0060 (6)
O1	0.0435 (7)	0.0375 (6)	0.0788 (9)	0.0060 (5)	0.0107 (6)	0.0213 (6)
C1	0.0364 (8)	0.0316 (7)	0.0411 (8)	0.0012 (6)	0.0024 (6)	0.0045 (6)
C2	0.0343 (8)	0.0307 (8)	0.0449 (9)	0.0040 (6)	0.0042 (6)	0.0069 (6)
C3	0.0366 (8)	0.0281 (7)	0.0381 (8)	0.0037 (6)	0.0015 (6)	0.0037 (6)
C11	0.0317 (7)	0.0280 (7)	0.0344 (7)	0.0002 (5)	−0.0015 (6)	−0.0006 (5)
C12	0.0380 (8)	0.0307 (7)	0.0435 (9)	−0.0009 (6)	0.0009 (7)	0.0039 (6)
C13	0.0491 (9)	0.0281 (7)	0.0433 (9)	0.0054 (7)	−0.0007 (7)	0.0027 (6)
C14	0.0385 (9)	0.0377 (9)	0.0436 (9)	0.0138 (7)	−0.0036 (7)	−0.0054 (7)
C15	0.0325 (8)	0.0482 (10)	0.0439 (9)	0.0033 (7)	0.0049 (7)	−0.0027 (7)
C16	0.0384 (8)	0.0310 (8)	0.0390 (8)	−0.0003 (6)	0.0012 (6)	0.0019 (6)
C22	0.0346 (8)	0.0281 (7)	0.0378 (8)	0.0057 (6)	0.0020 (6)	0.0003 (6)
C23	0.0389 (8)	0.0297 (8)	0.0427 (8)	0.0043 (6)	0.0069 (7)	0.0035 (6)
C24	0.0388 (9)	0.0383 (9)	0.0617 (11)	0.0002 (7)	0.0129 (8)	0.0033 (8)
C25	0.0344 (8)	0.0441 (10)	0.0679 (12)	0.0059 (7)	0.0082 (8)	−0.0067 (9)

Geometric parameters (Å, °)

S21—C22	1.7229 (14)	C15—C16	1.381 (2)
S21—C25	1.6960 (19)	C22—C23	1.379 (2)
F14—C14	1.3638 (19)	C23—C24	1.421 (2)
O1—C1	1.230 (2)	C24—C25	1.364 (3)
C1—C2	1.470 (2)	C2—H2	0.9500
C1—C22	1.474 (2)	C3—H3	0.9500
C2—C3	1.332 (2)	C12—H12	0.9500
C3—C11	1.467 (2)	C13—H13	0.9500
C11—C12	1.395 (2)	C15—H15	0.9500
C11—C16	1.403 (2)	C16—H16	0.9500
C12—C13	1.383 (2)	C23—H23	0.9500
C13—C14	1.375 (2)	C24—H24	0.9500
C14—C15	1.378 (2)	C25—H25	0.9500
S21···O1	2.9333 (14)	C14···H13^{ix}	2.9800
S21···C23^{i}	3.6512 (18)	C15···H25^{x}	3.0700
S21···C24^{i}	3.6843 (18)	C22···H23^{iv}	3.0600
S21···H23^{i}	3.1800	C23···H2	2.7400
F14···C25^{ii}	3.153 (2)	C25···H15^{xi}	2.9900
F14···H25^{ii}	2.4100	H2···C12	2.7600
O1···S21	2.9333 (14)	H2···C23	2.7400
O1···C16^{iii}	3.389 (2)	H2···H12	2.2100
O1···H3	2.4800	H2···H23	2.2800
O1···H3^{iii}	2.6600	H3···O1	2.4800
O1···H16^{iii}	2.5900	H3···H16	2.3700

C1···C24^{iv}	3.531 (2)	H3···O1^{iii}	2.6600
C15···C22^{v}	3.391 (2)	H12···C2	2.7600
C15···C23^{v}	3.561 (2)	H12···H2	2.2100
C16···O1^{iii}	3.389 (2)	H13···C13^{xii}	2.9600
C22···C23^{iv}	3.542 (2)	H13···C14^{xii}	2.9800
C22···C15^{v}	3.391 (2)	H15···C25^{x}	2.9900
C23···C22^{vi}	3.542 (2)	H15···H25^{x}	2.4500
C23···S21^{vii}	3.6512 (18)	H16···H3	2.3700
C23···C15^{v}	3.561 (2)	H16···O1^{iii}	2.5900
C24···C1^{vi}	3.531 (2)	H23···S21^{vii}	3.1800
C24···S21^{vii}	3.6843 (18)	H23···C2	2.8600
C25···F14^{viii}	3.153 (2)	H23···H2	2.2800
C1···H24^{iv}	3.1000	H23···C22^{vi}	3.0600
C2···H23	2.8600	H24···C1^{vi}	3.1000
C2···H12	2.7600	H25···F14^{viii}	2.4100
C12···H2	2.7600	H25···C15^{xi}	3.0700
C13···H13^{ix}	2.9600	H25···H15^{xi}	2.4500
C22—S21—C25	91.58 (8)	C23—C24—C25	112.18 (16)
O1—C1—C2	122.97 (15)	S21—C25—C24	112.84 (14)
O1—C1—C22	119.55 (14)	C1—C2—H2	120.00
C2—C1—C22	117.48 (14)	C3—C2—H2	120.00
C1—C2—C3	120.50 (16)	C2—C3—H3	117.00
C2—C3—C11	126.67 (16)	C11—C3—H3	117.00
C3—C11—C12	123.27 (14)	C11—C12—H12	119.00
C3—C11—C16	118.40 (15)	C13—C12—H12	119.00
C12—C11—C16	118.33 (15)	C12—C13—H13	121.00
C11—C12—C13	121.23 (15)	C14—C13—H13	121.00
C12—C13—C14	118.09 (16)	C14—C15—H15	121.00
F14—C14—C13	118.52 (15)	C16—C15—H15	121.00
F14—C14—C15	118.29 (14)	C11—C16—H16	119.00
C13—C14—C15	123.19 (16)	C15—C16—H16	119.00
C14—C15—C16	117.92 (15)	C22—C23—H23	124.00
C11—C16—C15	121.22 (16)	C24—C23—H23	124.00
S21—C22—C1	118.36 (10)	C23—C24—H24	124.00
S21—C22—C23	111.50 (11)	C25—C24—H24	124.00
C1—C22—C23	130.14 (14)	S21—C25—H25	124.00
C22—C23—C24	111.90 (15)	C24—C25—H25	124.00
C22—S21—C25—C24	0.36 (15)	C3—C11—C12—C13	178.06 (15)
C25—S21—C22—C1	−179.49 (13)	C16—C11—C12—C13	−1.6 (2)
C25—S21—C22—C23	−0.18 (13)	C12—C11—C16—C15	0.7 (2)
O1—C1—C2—C3	8.5 (3)	C11—C12—C13—C14	1.2 (2)
C22—C1—C2—C3	−172.22 (15)	C12—C13—C14—F14	179.75 (15)
O1—C1—C22—S21	−2.5 (2)	C12—C13—C14—C15	0.2 (3)
C2—C1—C22—C23	−1.0 (2)	F14—C14—C15—C16	179.39 (14)
O1—C1—C22—C23	178.34 (16)	C13—C14—C15—C16	−1.1 (3)

C2—C1—C22—S21	178.18 (11)	C14—C15—C16—C11	0.6 (2)
C1—C2—C3—C11	−179.24 (15)	S21—C22—C23—C24	−0.03 (18)
C2—C3—C11—C16	−177.36 (16)	C1—C22—C23—C24	179.17 (16)
C2—C3—C11—C12	3.0 (3)	C22—C23—C24—C25	0.3 (2)
C3—C11—C16—C15	−178.97 (14)	C23—C24—C25—S21	−0.4 (2)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*−1, *y*+1, *z*; (iii) −*x*, −*y*, −*z*+1; (iv) −*x*+1/2, *y*−1/2, −*z*+1/2; (v) −*x*, −*y*+1, −*z*+1; (vi) −*x*+1/2, *y*+1/2, −*z*+1/2; (vii) *x*, *y*+1, *z*; (viii) *x*+1, *y*−1, *z*; (ix) −*x*−1/2, *y*−1/2, −*z*+1/2; (x) *x*−1, *y*, *z*; (xi) *x*+1, *y*, *z*; (xii) −*x*−1/2, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1	0.95	2.48	2.822 (2)	101
C16—H16···O1^{iii}	0.95	2.59	3.389 (2)	142
C25—H25···F14^{viii}	0.95	2.41	3.153 (2)	135
C13—H13···Cg^{xii}	0.95	2.84	3.567 (2)	134

Symmetry codes: (iii) −*x*, −*y*, −*z*+1; (viii) *x*+1, *y*−1, *z*; (xii) −*x*−1/2, *y*+1/2, −*z*+1/2.

Fig. 1

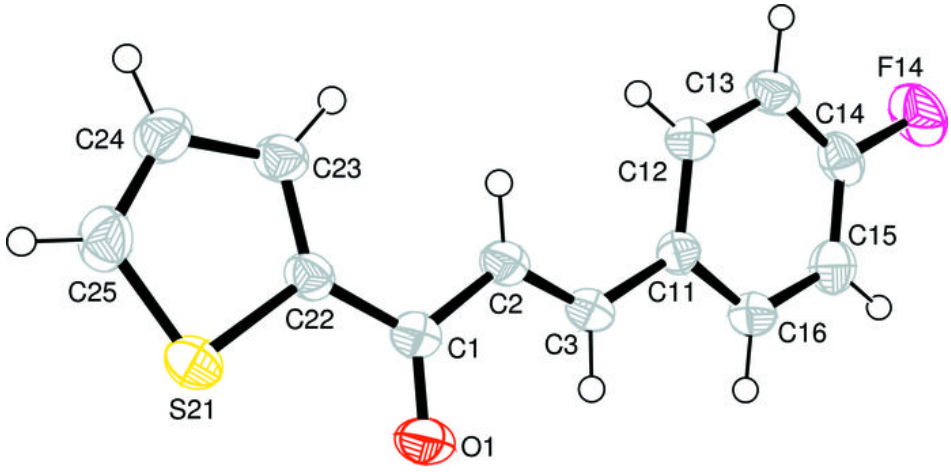

Fig. 2