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1-[2-Chloro-4-(4-fluorophenoxy)phenyl]-ethanone

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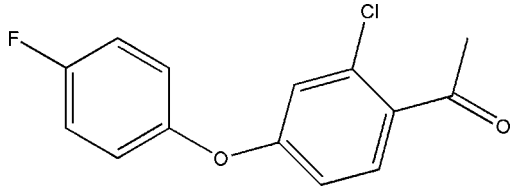
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.124; data-to-parameter ratio = 13.2.

The title compound, $C_{14}H_{10}ClFO_2$, was obtained in a search for new fluorine-containing compounds with improved biological activity. In the molecule, the two benzene rings make a dihedral angle of 67.45 (5)°. The crystal packing exhibits weak intermolecular C—H···Cl hydrogen bonds and π–π interactions between the aromatic rings of neighbouring molecules [centroid-to-centroid distance of 3.669 (6) Å; symmetry code: $-x, -y+1, -z+1$].

Related literature

For the crystal structure of a related compound, see: Kartal *et al.* (2006). For details of the biological activities of fluorine-containing compounds, see: Billard & Langlois (2002).



Experimental

Crystal data

$C_{14}H_{10}ClFO_2$
M_r = 264.67
Monoclinic, $P2_1/c$
a = 11.060 (2) Å
b = 10.660 (2) Å
c = 10.489 (2) Å
β = 97.91 (3)°
V = 1224.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 293 (2) K
0.22 × 0.16 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.934, T_{max} = 0.957
3859 measured reflections
2158 independent reflections
1766 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.124
S = 1.06
2158 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···Cl1^{i}	0.93	2.84	3.730 (3)	160

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

Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2262).

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Rigaku (2001). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.

supplementary materials

Acta Cryst. (2007). E**63**, o3243 [**doi:10.1107/S160053680702836X**]

1-[2-Chloro-4-(4-fluorophenoxy)phenyl]ethanone

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Comment

The fluorinated organic products exhibit unique properties that are of great interest for a variety of applications (Billard & Langlois, 2002). In a search for new fluorine-containing compounds with better biological activity, the title compound, (I) (Fig. 1), was synthesized. We report here its crystal structure.

Atom F1 lies 0.005 Å out of the mean plane of benzene ring C8/C10/C12/C14–C16. Two benzene rings make a dihedral angle of 67.45 (5) Å. As can be seen from the packing diagram (Fig. 2), the crystal structure of (I) is stabilized by weak intermolecular C—H···Cl hydrogen bonds (Table 1) and a π-π stacking interactions, proved by the short distance $Cg1\cdots Cg1^{ii}$ of 3.669 (6) Å, where *Cg*1 is a centroid of C2–C7 [symmetry code: (ii) $-x, 1-y, 1-z$].

Experimental

Acetyl chlorid (10 mmol) was added dropwise to the solution of 1-(3-chlorophenoxy)-4-fluorobenzene (10 mmol), aluminium oxide (13 mmol), carbon sulfide (20 ml) and the mixture was heated under reflux for 1 h. Then the mixture was extracted with CS_2 (15 ml) and the organic layer was washed with 50% NaOH solution and water. The excess CS_2 was removed on a water vacuum pump to obtain the final product (85% yield). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2 (1.5 for methyl group) times U_{eq}(C).

Figures

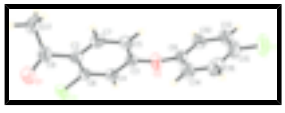

Fig. 1. View of the title compound (I), with displacement ellipsoids drawn at the 40% probability level.

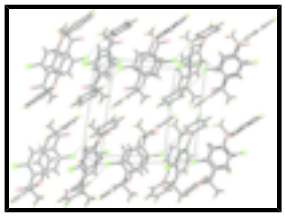

Fig. 2. A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

1-[2-Chloro-4-(4-fluorophenoxy)phenyl]ethanone

Crystal data

$C_{14}H_{10}ClFO_2$	F_{000} = 544
M_r = 264.67	D_x = 1.435 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1167 reflections
a = 11.060 (2) Å	θ = 2.3–19.5º
b = 10.660 (2) Å	μ = 0.31 mm^{-1}
c = 10.489 (2) Å	T = 293 (2) K
β = 97.91 (3)º	Block, colourless
V = 1224.8 (4) Å^3	0.22 × 0.16 × 0.14 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer	2158 independent reflections
Radiation source: Rotating anode	1766 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 293(2) K	θ_{max} = 25.0º
ω oscillation scans	θ_{min} = 2.7º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −13→13
T_{min} = 0.934, T_{max} = 0.957	k = −12→11
3859 measured reflections	l = −12→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.124	$w = 1/[\sigma^2(F_o^2) + (0.0689P)^2 + 0.2598P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
2158 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
164 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
Cl1	0.04538 (6)	0.47347 (7)	0.20376 (6)	0.0681 (2)
O2	−0.23410 (13)	0.64987 (15)	0.48929 (16)	0.0603 (4)
C2	0.11898 (18)	0.6452 (2)	0.39413 (19)	0.0466 (5)
C3	−0.11690 (17)	0.65749 (19)	0.45893 (19)	0.0444 (5)
C4	−0.09306 (18)	0.5813 (2)	0.35886 (19)	0.0459 (5)
H4A	−0.1551	0.5338	0.3134	0.055*
C5	−0.02607 (18)	0.7276 (2)	0.5271 (2)	0.0497 (5)
H5A	−0.0428	0.7795	0.5938	0.060*
C6	0.02389 (18)	0.5766 (2)	0.32717 (18)	0.0453 (5)
C7	0.09043 (18)	0.7198 (2)	0.4950 (2)	0.0496 (5)
H7A	0.1523	0.7659	0.5425	0.060*
C8	−0.28365 (17)	0.7520 (2)	0.5473 (2)	0.0473 (5)
C9	0.2472 (2)	0.6428 (2)	0.3621 (2)	0.0616 (6)
C10	−0.34782 (18)	0.7252 (2)	0.6465 (2)	0.0574 (6)
H10A	−0.3517	0.6434	0.6764	0.069*
O1	0.26739 (17)	0.6348 (3)	0.25168 (19)	0.0985 (8)
C12	−0.4064 (2)	0.8204 (3)	0.7014 (2)	0.0726 (8)
H12A	−0.4512	0.8038	0.7683	0.087*
F1	−0.45471 (15)	1.03643 (19)	0.7133 (2)	0.1115 (7)
C14	−0.2778 (2)	0.8714 (2)	0.5009 (2)	0.0632 (6)
H14A	−0.2349	0.8879	0.4324	0.076*
C15	−0.3982 (2)	0.9394 (3)	0.6567 (3)	0.0720 (8)
C16	−0.3362 (2)	0.9672 (3)	0.5569 (3)	0.0738 (7)
H16A	−0.3332	1.0492	0.5270	0.089*
C17	0.3492 (2)	0.6478 (3)	0.4714 (3)	0.0733 (7)
H17A	0.4259	0.6479	0.4382	0.110*
H17B	0.3450	0.5760	0.5257	0.110*
H17C	0.3423	0.7229	0.5204	0.110*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Cl1	0.0814 (4)	0.0733 (5)	0.0526 (4)	0.0182 (3)	0.0196 (3)	−0.0135 (3)
O2	0.0508 (8)	0.0595 (10)	0.0752 (11)	−0.0078 (7)	0.0255 (8)	−0.0161 (8)
C2	0.0459 (11)	0.0493 (13)	0.0453 (11)	0.0077 (9)	0.0081 (9)	0.0099 (9)
C3	0.0432 (10)	0.0465 (12)	0.0454 (11)	0.0020 (8)	0.0134 (8)	0.0020 (9)
C4	0.0479 (11)	0.0486 (13)	0.0408 (10)	0.0019 (9)	0.0046 (8)	−0.0032 (9)
C5	0.0558 (12)	0.0500 (13)	0.0449 (11)	0.0009 (10)	0.0125 (9)	−0.0080 (9)
C6	0.0519 (11)	0.0479 (12)	0.0369 (10)	0.0127 (9)	0.0098 (8)	0.0032 (9)
C7	0.0480 (11)	0.0507 (13)	0.0495 (11)	−0.0041 (9)	0.0045 (9)	0.0010 (10)
C8	0.0402 (10)	0.0562 (14)	0.0469 (11)	0.0018 (9)	0.0109 (8)	−0.0052 (9)
C9	0.0517 (13)	0.0691 (16)	0.0670 (15)	0.0070 (11)	0.0189 (11)	0.0144 (12)
C10	0.0489 (12)	0.0712 (16)	0.0547 (13)	−0.0045 (11)	0.0162 (10)	0.0006 (11)
O1	0.0658 (11)	0.164 (2)	0.0713 (13)	0.0140 (12)	0.0300 (10)	0.0212 (13)
C12	0.0534 (14)	0.108 (2)	0.0603 (15)	0.0007 (14)	0.0224 (11)	−0.0166 (15)
F1	0.0795 (11)	0.1223 (16)	0.1327 (17)	0.0351 (10)	0.0143 (11)	−0.0616 (13)
C14	0.0630 (14)	0.0650 (17)	0.0650 (15)	0.0024 (11)	0.0207 (12)	0.0060 (12)
C15	0.0464 (12)	0.087 (2)	0.0813 (18)	0.0167 (12)	0.0043 (12)	−0.0316 (16)
C16	0.0645 (15)	0.0604 (17)	0.095 (2)	0.0124 (12)	0.0042 (14)	−0.0005 (14)
C17	0.0458 (13)	0.086 (2)	0.0873 (19)	0.0005 (12)	0.0066 (12)	0.0068 (15)

Geometric parameters (Å, °)

Cl1—C6	1.739 (2)	C9—O1	1.213 (3)
O2—C3	1.379 (2)	C9—C17	1.494 (4)
O2—C8	1.396 (2)	C10—C12	1.373 (3)
C2—C6	1.390 (3)	C10—H10A	0.9300
C2—C7	1.394 (3)	C12—C15	1.359 (4)
C2—C9	1.501 (3)	C12—H12A	0.9300
C3—C5	1.372 (3)	F1—C15	1.384 (3)
C3—C4	1.381 (3)	C14—C16	1.383 (3)
C4—C6	1.380 (3)	C14—H14A	0.9300
C4—H4A	0.9300	C15—C16	1.361 (4)
C5—C7	1.378 (3)	C16—H16A	0.9300
C5—H5A	0.9300	C17—H17A	0.9600
C7—H7A	0.9300	C17—H17B	0.9600
C8—C14	1.367 (3)	C17—H17C	0.9600
C8—C10	1.368 (3)		
C3—O2—C8	119.52 (16)	O1—C9—C2	121.3 (2)
C6—C2—C7	116.67 (18)	C17—C9—C2	117.7 (2)
C6—C2—C9	123.4 (2)	C8—C10—C12	119.3 (2)
C7—C2—C9	120.0 (2)	C8—C10—H10A	120.4
C5—C3—O2	123.77 (18)	C12—C10—H10A	120.4
C5—C3—C4	120.93 (18)	C15—C12—C10	119.2 (2)
O2—C3—C4	115.14 (18)	C15—C12—H12A	120.4
C6—C4—C3	119.21 (19)	C10—C12—H12A	120.4
C6—C4—H4A	120.4	C8—C14—C16	119.2 (2)
C3—C4—H4A	120.4	C8—C14—H14A	120.4
C3—C5—C7	118.8 (2)	C16—C14—H14A	120.4
C3—C5—H5A	120.6	C12—C15—C16	122.2 (2)
C7—C5—H5A	120.6	C12—C15—F1	119.6 (3)

C4—C6—C2	121.89 (19)	C16—C15—F1	118.2 (3)
C4—C6—Cl1	115.53 (17)	C15—C16—C14	118.7 (3)
C2—C6—Cl1	122.51 (15)	C15—C16—H16A	120.6
C5—C7—C2	122.5 (2)	C14—C16—H16A	120.6
C5—C7—H7A	118.8	C9—C17—H17A	109.5
C2—C7—H7A	118.8	C9—C17—H17B	109.5
C14—C8—C10	121.4 (2)	H17A—C17—H17B	109.5
C14—C8—O2	122.00 (19)	C9—C17—H17C	109.5
C10—C8—O2	116.4 (2)	H17A—C17—H17C	109.5
O1—C9—C17	121.0 (2)	H17B—C17—H17C	109.5
C8—O2—C3—C5	30.6 (3)	C3—O2—C8—C10	−137.2 (2)
C8—O2—C3—C4	−154.03 (19)	C6—C2—C9—O1	35.9 (4)
C5—C3—C4—C6	−0.3 (3)	C7—C2—C9—O1	−143.7 (3)
O2—C3—C4—C6	−175.84 (19)	C6—C2—C9—C17	−142.9 (2)
O2—C3—C5—C7	174.4 (2)	C7—C2—C9—C17	37.5 (3)
C4—C3—C5—C7	−0.7 (3)	C14—C8—C10—C12	−0.7 (3)
C3—C4—C6—C2	0.8 (3)	O2—C8—C10—C12	−175.2 (2)
C3—C4—C6—Cl1	177.70 (16)	C8—C10—C12—C15	−0.7 (4)
C7—C2—C6—C4	−0.2 (3)	C10—C8—C14—C16	1.1 (4)
C9—C2—C6—C4	−179.8 (2)	O2—C8—C14—C16	175.4 (2)
C7—C2—C6—Cl1	−176.91 (15)	C10—C12—C15—C16	1.7 (4)
C9—C2—C6—Cl1	3.5 (3)	C10—C12—C15—F1	−178.6 (2)
C3—C5—C7—C2	1.4 (3)	C12—C15—C16—C14	−1.3 (4)
C6—C2—C7—C5	−0.9 (3)	F1—C15—C16—C14	179.0 (2)
C9—C2—C7—C5	178.7 (2)	C8—C14—C16—C15	−0.2 (4)
C3—O2—C8—C14	48.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14A···Cl1^{i}	0.93	2.84	3.730 (3)	160

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2.

Fig. 1

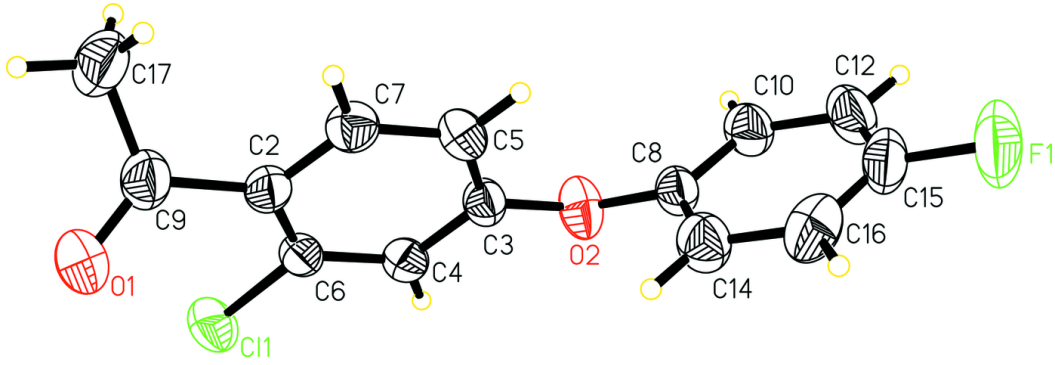

Fig. 2