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1-(2,4-Dichloro-5-fluorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.030
wR factor = 0.078
Data-to-parameter ratio = 13.9

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

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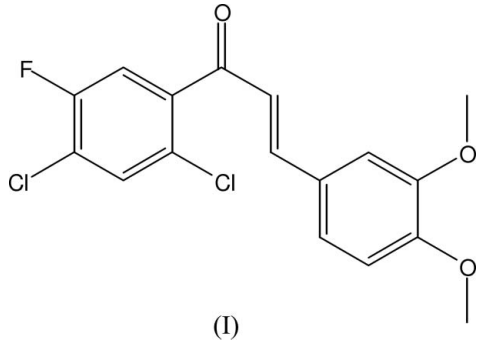
In the title biologically active compound, $C_{17}H_{13}Cl_2FO_3$, the central C=C double bond is *trans* configured. The molecule consists of two essentially planar parts which are twisted by 67.06 (2)° with respect to each other.

Comment

Among various organic compounds reported for their non-linear optical (NLO) properties, chalcone derivatives are notable for their excellent blue-light transmittance and good crystallizability (Uchida *et al.*, 1998). They provide a necessary molecular electronic configuration to show NLO effects, with two aromatic rings connected through a conjugated bridge (Goto *et al.*, 1991; Tam *et al.*, 1989; Indira *et al.*, 2002). Substitution on either of the benzene rings appears to increase the likelihood of noncentrosymmetric crystal packing, as well as enhancing the electronic properties of the molecule (Fichou *et al.*, 1988). The crystal structures of 3-(3,4-dimethoxyphenyl)-1-(4-fluorophenyl)prop-2-en-1-one (Butcher *et al.*, 2006), 4′-fluorochalcone (Ng *et al.*, 2006), 1-(2,4-dichlorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Patil *et al.*, 2006) and 1-(4-fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (Harrison *et al.*, 2006) have been reported. Recently, fluorinated organic compounds have attracted attention due to the ability of fluorine to act as a polar hydrogen or hydroxyl mimic. Therefore, substitution of hydrogen by fluorine has been a strategy in designing molecules for biological activity studies (Holla *et al.*, 2004). Crystal structures of fluorinated chalcones are relatively rare in the literature. In this context, the present work reports the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Crystallographic Database, Version 5.27, November 2005 updated May 2006; *MOGUL* Version 1.1; Allen, 2002). The central C=C double bond is *trans* configured. The molecule

consists of two planar segments which are twisted by 67.06 (2)° with respect to each other. One of these is the 3,4-(dimethoxy)benzene group, which is coplanar with the propenone group (r.m.s. deviation for all non H atoms = 0.046 Å), while the other is the halogenated phenyl ring. All torsion angles are close to 0 and 180°; only those about the C1—C11 bond differ significantly from planarity (Table 1).

The crystal packing reveals two weak C—H···O contacts (Table 2).

Experimental

The title compound was synthesized according to the method reported in the literature by Furniss *et al.* (1989), in a yield of 75%. The compound was purified by recrystallization from ethanol. Crystal growth was carried out in acetone solvent by the slow evaporation technique (m.p. 386–388 K). Analysis for (I): found (calculated) C 57.40 (57.49%), H 3.67 (3.69%).

Crystal data

$C_{17}H_{13}Cl_2FO_3$
M_r = 355.17
Monoclinic, $P2_1/c$
a = 6.8572 (5) Å
b = 16.7211 (11) Å
c = 13.9299 (12) Å
β = 98.173 (6)°
V = 1581.0 (2) Å^3
Z = 4
D_x = 1.492 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 173 (2) K
Block, colourless
0.48 × 0.46 × 0.43 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.819, T_{max} = 0.836
11672 measured reflections
2940 independent reflections
2728 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.078
S = 1.06
2940 reflections
211 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.6433P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0178 (15)

Table 1
Selected torsion angles (°).

O1—C1—C11—C12	63.1 (2)	O1—C1—C11—C16	−115.03 (16)
C2—C1—C11—C12	−118.54 (15)	C2—C1—C11—C16	63.35 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O27^{i}	0.95	2.50	3.3067 (17)	143
C16—H16···O28^{i}	0.95	2.43	3.3072 (17)	154

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

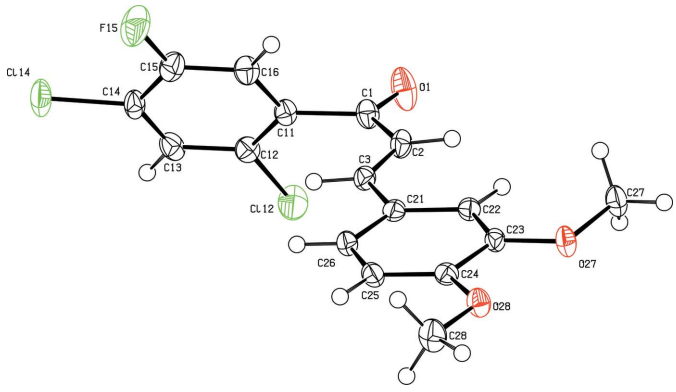


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

H atoms were found in a difference map, but were placed geometrically and allowed to ride on their parent C atoms at distances of 0.95 and 0.98 Å for aromatic and methyl groups, respectively, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}). The methyl groups were allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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