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3-(1,3-Benzodioxol-5-yl)-2-bromo-1-(2,4-dichloro-5-fluorophenyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.083
Data-to-parameter ratio = 17.3

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

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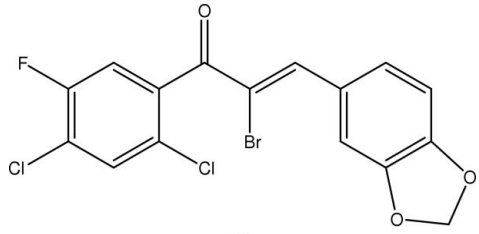
In the title molecule, $C_{16}H_8BrCl_2FO_3$, the dioxole ring adopts a twist conformation. The molecules are linked into a chain along the c axis by C—H···O intermolecular interactions, and adjacent chains are crosslinked *via* π–π interactions.

Comment

Chalcone and its derivatives are an important class of chemical compounds which are being studied extensively because of their nonlinear optical properties (Kitaoka *et al.*, 1990). In addition, many of the chalcones exhibit antiplasmodial activity (Go *et al.*, 2004). We report here the crystal structure of the title chalcone derivative, (I).



(I)

Bond lengths and angles in (I) have normal values (Allen *et al.*, 1987) and are comparable to those observed in 3-[4-(methylsulfanyl)phenyl]-1-(4-nitrophenyl)prop-2-en-1-one (Harrison *et al.*, 2006). The dioxole ring adopts a twist conformation with Cremer & Pople (1975) puckering parameters q_2 and φ of 0.074 (3) Å and 155 (2)°, respectively. The dihedral angle between the two benzene rings is 66.6 (1)°. Atoms Cl1, Cl2 and F1 deviate by 0.070 (1), 0.041 (1) and 0.039 (2) Å, respectively, from the benzene ring to which they are attached.

A weak C11—H11···Br1 hydrogen-bonding interaction is observed in the molecular structure. The molecules are linked into a chain along the c axis by C—H···O intermolecular interactions (Table 1). A π–π interaction involving the C1–C6 (centroid $Cg1$) and C10–C15 (centroid $Cg2$) benzene rings in adjacent chains is observed, with a $Cg1\cdots Cg2^{ii}$ distance of 3.581 (1) Å [symmetry code: (ii) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$].

Experimental

3-(1,3-Benzodioxol-5-yl)-1-(2,4-dichloro-5-fluorophenyl)prop-2-en-1-one was prepared according to the literature procedure (Shivarama Holla *et al.*, 2006). To a solution of 3-(1,3-benzodioxol-5-yl)-1-(2,4-dichloro-5-fluorophenyl)prop-2-en-1-one (1 mmol) in chloroform (25 ml), bromine (1 mmol) was added slowly and the reaction mixture was stirred for 24 h. Excess chloroform was distilled off and

the precipitated 3-(1,3-benzodioxol-5-yl)-2,3-dibromo-1-(2,4-dichloro-5-fluorophenyl) propan-1-one was filtered off and dried. A mixture of dibromopropanone (1 mmol) and triethylamine (1 mmol) in dry benzene (35 ml) was stirred for 24 h. The content of the reaction mixture was filtered and the excess of solvent was removed under reduced pressure to obtain the title compound. Single crystals of (I) were grown by slow evaporation of an acetone solution.

Crystal data

$C_{16}H_8BrCl_2FO_3$
M_r = 418.03
Monoclinic, $P2_1/c$
a = 9.9442 (6) Å
b = 13.9545 (9) Å
c = 11.0593 (7) Å
β = 91.130 (1)°
V = 1534.36 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.05 mm^{-1}
T = 293 (2) K
0.23 × 0.22 × 0.21 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
17013 measured reflections
3590 independent reflections
2994 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.083
S = 1.00
3590 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O1^{i}	0.93	2.49	3.356 (3)	155
C11—H11···Br1	0.93	2.71	3.271 (2)	119

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

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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 *PARST* (Nardelli, 1995).

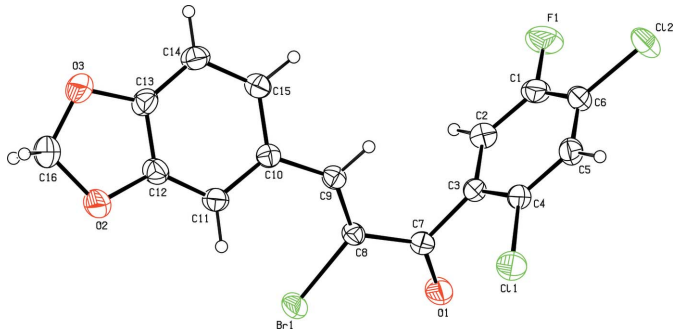


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammee, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2001). *SMART* (Version 5.625/NT/2000) and *SAINT* (Version 6.28a). Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Go, M.-L., Liu, M., Wilairat, P., Rosenthal, P. J., Saliba, K. J. & Kirk, K. (2004). *Antimicrob. Agents Chemother.* **48**, 3241–3245.
Harrison, W. T. A., Yathirajan, H. S., Mithun, A., Narayana, B. & Sarojini, B. K. (2006). *Acta Cryst.* E**62**, o4508–o4509.
Kitaoka, Y., Sasaki, T., Nakai, S., Yokotani, A., Goto, Y. & Nakayama, M. (1990). *Appl. Phys. Lett.* **56**, 2074–2076.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shivarama Holla, B., Sooryanarayana Rao, B., Sarojini, B. K., Akberali, P. M. & Suchetha Kumari, N. (2006). *Eur. J. Med. Chem.* **41**, 657–663.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.