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2-Bromo-1-(2,4-dichloro-5-fluorophenyl)-3-phenylprop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.077
Data-to-parameter ratio = 17.8

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

The molecular geometry of the title compound, $C_{15}H_8BrCl_2FO$, is stabilized by a C—H···Br interaction.

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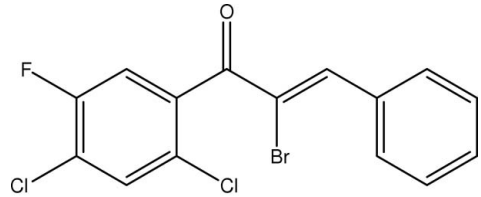
Comment

Chalcone derivatives have nonlinear optical (NLO) properties with good blue light transmittance. They also have a wide range of biological applications, such as anticancer (Rao *et al.*, 2004) and anti-inflammatory activity (Hsieh *et al.*, 2000). In view of the optical and medicinal importance of chalcone derivatives, we have prepared the title compound.



(I)

The geometric parameters of (I) lie within their expected ranges (Allen *et al.*, 1987). The dihedral angle between the two benzene rings is 89.1 (2)°. The O1—C7—C8—Br1 torsion angle is 17.4 (4)°. The molecular conformation is stabilized by a C—H···Br interaction (Table 1).

Experimental

1-(2,4-Dichloro-5-fluorophenyl)-3-phenylprop-2-en-1-one (1 mmol) was prepared by a literature procedure (Shivarama Holla *et al.*, 2006). To a solution of 1-(2,4-dichloro-5-fluorophenyl)-3-phenylprop-2-en-1-one) (1 mmol) in chloroform (25 ml), bromine (1 mmol) was added slowly with stirring. After the completion of addition of bromine (1 mmol), the reaction mixture was stirred for 24 h. Excess of chloroform was distilled off and precipitated 2,3-dibromo-1-(2,4-dichloro-5-fluorophenyl)-3-phenylpropan-1-one was filtered off and dried. A mixture of dibromopropanone (1 mmol) and triethylamine (1 mmol) in dry benzene (30 ml) was stirred for 24 h. The excess of solvent when removed under reduced pressure gave the title compound. It was crystallized from acetone by slow evaporation.

Crystal data

$C_{15}H_8BrCl_2FO$
M_r = 374.02
Monoclinic, Pc
a = 6.5423 (8) Å
b = 14.3317 (16) Å
c = 7.8040 (9) Å
β = 93.284 (2)°
V = 730.52 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.18 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
7433 measured reflections
3234 independent reflections
2946 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.077$
$S = 0.93$
3234 reflections
182 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}
Absolute structure: Flack (1983), 1526 Friedel pairs
Flack parameter: 0.049 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···Br1	0.93	2.74	3.319 (3)	122

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H = 0.93 Å and with U_{iso}(H) = 1.5U_{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).

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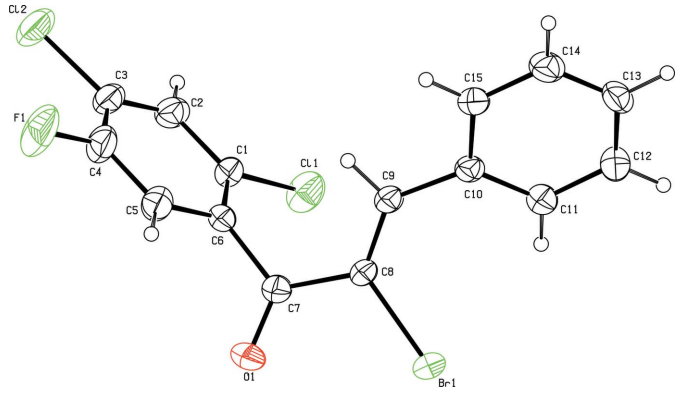

Figure 1
The molecular structure of the title compound showing 30% probability displacement ellipsoids.

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