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2-Bromo-3-(4-chlorophenyl)-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) = 0.004 Å
R factor = 0.039
wR factor = 0.106
Data-to-parameter ratio = 18.8

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

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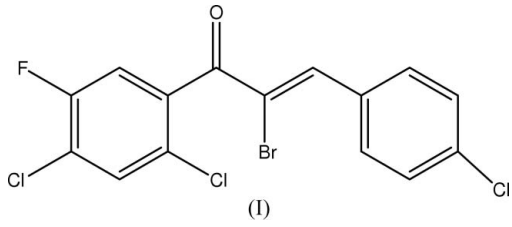
The title compound, $C_{15}H_7BrCl_3FO$, crystallizes with two molecules in the asymmetric unit. The molecular conformation is stabilized by C—H···Br intramolecular interactions.

Comment

Chalcones are an important class of compounds that occur in edible plants. They have a wide variety of pharmaceutical activities including anticancer (Modzelewska *et al.*, 2006), anti-inflammatory (Won *et al.*, 2005) and antipyretic (De Leon *et al.*, 2003). Some chalcones show antiplasmodial (Go *et al.*, 2004) activity. If chalcones crystallize in a non-centrosymmetric space group they can be used as a non-linear optical device for second-harmonic generation. In view of the above, we have undertaken the X-ray crystal structure determination of the title compound (I).



(I)

Bond lengths and bond angles of the title compound are comparable those in reported structures (Harrison *et al.*, 2006). The dihedral angle between the two benzene rings in one molecule is 87.2 (1)° (C1–C6 and C10–C15) and in the other molecule is 83.5 (1)° (C16–C21 and C25–C30). The O1—C7—C8—Br1 torsion angle is −4.1 (4)° in one molecule and 0.2 (4)° (O2—C22—C23—Br2) in the other.

The molecular conformation is stabilized by C—H···Br (Table 1) intramolecular interactions. An analysis of the crystal structure of (I) with *PLATON* (Spek, 2003) indicates no significant intermolecular hydrogen bonds.

Experimental

3-(4-Chlorophenyl)-1-(2,4-dichloro-5-fluorophenyl)prop-2-en-1-one was prepared by a literature procedure (Shivarama Holla *et al.*, 2006). To a solution of propenone (1 mmol) in chloroform (25 ml), bromine (1 mmol) was added slowly with stirring and the reaction mixture was then stirred for 24 h. Excess chloroform was distilled off and the precipitated 2,3-dibromo-3-(4-chlorophenyl)-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 (1 mmol) was stirred for 24 h. The excess solvent was removed under reduced pressure, giving the title compound which was recrystallized from chloroform by slow evaporation.

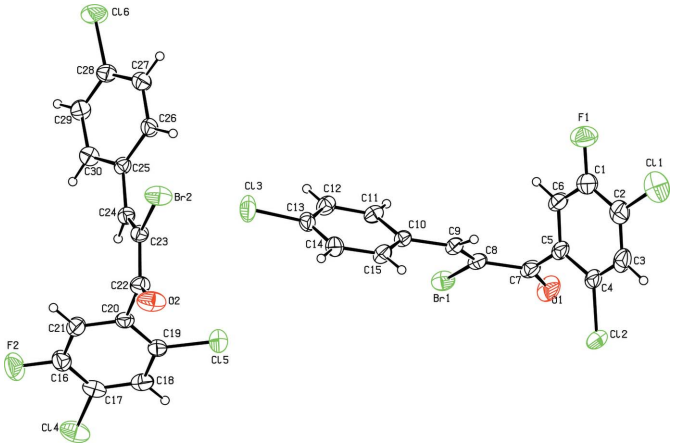


Figure 1
The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids.

Crystal data

$C_{15}H_7BrCl_3FO$
M_r = 408.46
Orthorhombic, *Pbca*
a = 14.3752 (9) Å
b = 11.3099 (7) Å
c = 37.302 (2) Å
V = 6064.6 (6) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 3.24 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
49754 measured reflections
7133 independent reflections
4962 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.00
7133 reflections
379 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···Br1	0.93	2.89	3.297 (3)	108
C26—H26···Br2	0.93	2.67	3.246 (3)	121

H atoms were positioned geometrically and were treated as riding, with C—H = 0.93 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).

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