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2,3-Dibromo-3-(4-chlorophenyl)-1-(2,4-dichloro-5-fluorophenyl)propan-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.041
wR factor = 0.133
Data-to-parameter ratio = 20.3

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

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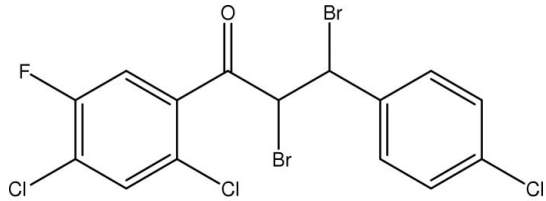
The title compound, $C_{15}H_8Br_2Cl_3FO$, crystallizes with two independent molecules in the asymmetric unit. The dihedral angle between the two benzene rings is 58.0 (2)° in one molecule and 52.0 (2)° in the other. A C—H···Cl intramolecular interaction is observed. The crystal packing is stabilized by van der Waals interactions.

Comment

Chalcone derivatives exhibit beneficial biological activities including anti-inflammatory (Hsieh *et al.*, 2000), antipyretic (De Leon *et al.*, 2003), anti-invasive (Mukherjee *et al.*, 2001), antiproliferative (Lin *et al.*, 2002) and antitumor activities (Saydam *et al.*, 2003). Furthermore, many chalcone derivatives exhibit excellent nonlinear optical (NLO) properties. We report here the crystal structure of the title compound, (I).



(I)

The asymmetric unit of the title compound contains two independent molecules (Fig. 1), which have slightly different orientations for the benzene rings [C7—C8—C9—C10 = 166.0 (4)° and C22—C23—C24—C25 = 154.3 (4)°]. The dihedral angle between the two benzene rings (C1–C6 and C10–C15) is 58.0 (2)° in one molecule, and 52.0 (2)° in the other molecule (C16–C21 and C25–C30). Bond lengths and angles in (I) are normal and comparable to those found in a similar structure (Harrison *et al.*, 2006).

A weak C—H···Cl (Table 1) intramolecular interaction is observed in one of the independent molecules. The crystal packing is stabilized by van der Waals interactions.

Experimental

3-(4-Chlorophenyl)-1-(2,4-dichloro-5-fluorophenyl)prop-2-en-1-one was prepared according to the literature procedure of Shivarama Holla *et al.* (2006). To a solution of 3-(4-chlorophenyl)-1-(2,4-dichloro-5-fluorophenyl)prop-2-en-1-one (1 mmol) in chloroform (25 ml), bromine (1 mmol) was added slowly with stirring and the reaction mixture was stirred for 24 h. Excess chloroform was distilled off and the precipitated compound (I) was filtered off and dried. It was recrystallized from chloroform by slow evaporation.

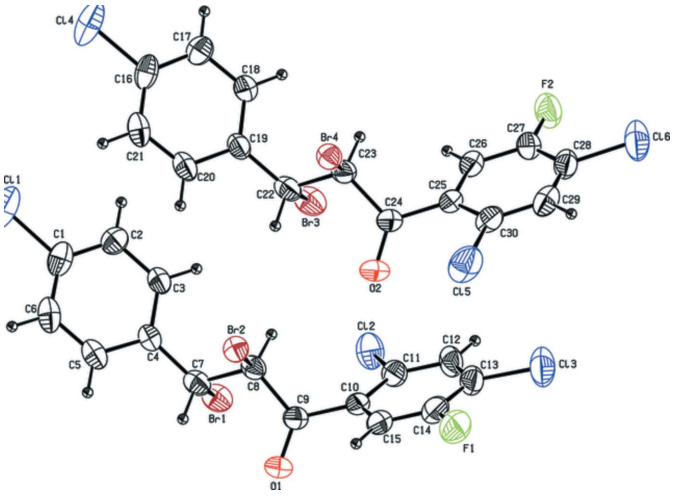


Figure 1
The asymmetric unit of (I), showing 30% probability displacement ellipsoids.

Crystal data

$C_{15}H_8Br_2Cl_3FO$
M_r = 489.38
Monoclinic, $P2_1/c$
a = 10.5292 (10) Å
b = 10.5897 (10) Å
c = 30.534 (3) Å
β = 91.111 (2)°
V = 3403.9 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 5.24 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
38185 measured reflections
8041 independent reflections
4658 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.133
S = 0.93
8041 reflections
397 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···Cl2	0.98	2.77	3.363 (4)	120

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 or 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C). The components of the displacement parameters in the direction of the C—Br bonds were restrained to be equal.

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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