3-(Biphenyl-4-yl)-2,3-dibromo-1-(2,4-dichlorophenyl)propan-1-one

The two aromatic rings of the biphenyl group of the title compound, C21H14Br2Cl2O, are not coplanar and the carbonyl group is twisted out of the plane of the adjacent dichlorophenyl ring. The crystal packing is stabilized by C—H···O and C—H···Br contacts.

Comment

For a structurally simple group of compounds, chalcones display an impressive array of biological activities, among which antimalarial (Liu et al., 2003), antiprotozoal (Nielsen et al., 1998), nitric oxide inhibition (Rajas et al., 2002) and anticancer activities (Dinkova-Kostova et al., 1998) have been reported in the literature. Among several organic compounds reported for non-linear optical (NLO) properties, chalcone derivatives are notable materials for their excellent blue light transmittance and good crystallizability. They provide a necessary configuration to show NLO properties, with two planar rings connected through a conjugated double bond (Goto et al., 1991; Uchida et al., 1998; Tam et al., 1989; Indira et al., 2002, Sarojini et al., 2006).

The substitution of a bromo group on either of the phenyl rings greatly influences the non-centrosymmetric crystal packing. The bromo group can obviously improve the molecular first-order hyperpolarizabilities and can effectively reduce dipole–dipole interactions between the molecules. Chalcone derivatives usually have a lower melting temperature, which can be a drawback when we use these crystals in optical instruments. Chalcone dibromides usually have higher melting points and are thermally stable. Only a few structures of these compounds have been reported (Butcher, Yathirajan, Anilkumar et al., 2006; Butcher, Yathirajan, Sarojini et al., 2006; Harrison et al., 2005). As a continuation of our studies on chalcones and their derivatives (Yathirajan et al., 2006, and references therein), a chalcone dibromide, (I), was prepared by the bromination of chalcone [(2E)-3-(biphenyl-4-yl)-1-(2,4-dichlorophenyl)prop-2-en-1-one].

A perspective view of (I) is shown in Fig. 1. The two aromatic rings of the biphenyl residue are not coplanar [dihedral angle = 30.67 (9)°]. The carbonyl group is twisted out...
of the plane of the adjacent dichlorophenyl ring (Table 1). The Br—C—C—Br unit adopts an almost perfect antiperiplanar conformation (Table 1). There are no classical hydrogen bonds, but the crystal packing is stabilized by C—H···O and C—H···Br contacts (Table 2).

Experimental

Chalcone [(2E)-3-(biphenyl-4-yl)-1-(2,4-dichlorophenyl)prop-2-en-1-one] (3.52 g, 0.01 mol) was treated with bromine in acetic acid (30%) until the orange colour of the solution persisted. After stirring for half an hour, the contents were poured on to crushed ice. The resulting solid mass was collected by filtration. The compound was dried and recrystallized from ethanol. Crystals suitable for a structure determination were obtained from an acetone and toluene (1:1) mixture by slow evaporation (yield 82%; m.p. 453–455 K). Analysis for C$_2$H$_4$Br$_2$Cl$_2$O found (calculated): C 49.03 (49.16), H 2.69% (2.75%).

Figure 1

The molecular structure of the title compound, showing the atom numbering and displacement ellipsoids drawn at the 50% probability level.

Table 1

Selected torsion angles (°).

| C1—C2—C3—C21 | 174.25 (18) | O1—C1—C11—C12 | 41.0 (4) |
| Br1—C2—C3—Br2 | 179.19 (9) | O1—C11—C11—C16 | −131.8 (3) |

Table 2

Hydrogen-bond geometry (Å, °).

| D—H···A | D—H | H···A | D···A | D—H···A |
| C15—H15—O1i | 0.95 | 2.57 | 3.188 (3) | 123 |
| C16—H16—O1ii | 0.95 | 2.60 | 3.211 (3) | 123 |
| C32—H32—O1iv | 0.95 | 2.54 | 3.482 (3) | 172 |
| C23—H23—Br1v | 0.95 | 2.92 | 3.862 (2) | 172 |

Symmetry codes: (i) $x, y + rac{1}{2}, z + rac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 2$; (iii) $-x + 1, -y + 1, -z + 1$.

H atoms were found in a difference map, but they were refined using a riding model, with C—H = 0.95 Å for aromatic and C—H = 1.00 Å for tertiary H atoms. $U_{eq}(H)$ values were set at 1.2$U_{eq}$(C). The deepest residual electron-density hole is located 0.69 Å from atom Br2.

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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References


Crystal data

C$_2$H$_4$Br$_2$Cl$_2$O

Monoclinic, $P2_1/c$

$\alpha = 18.1156$ (9) Å

$\beta = 100.762$ (4) Å

$V = 1887.35$ (17) Å$^3$

Data collection

Stoe IPDS-II two-circle diffractometer

$\omega$ scans

Absorption correction: multi-scan

(MULABS; Spek, 2003, Blessing, 1995)

$T_{max} = 0.259, T_{min} = 0.335$

Refinement

Refinement on $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.091$

$S = 1.06$

$5863$ reflections

$236$ parameters

H-atom parameters constrained

Extinction correction: SHELXL97

Extinction coefficient: 0.0083 (5)