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1-(4-Bromophenyl)-3-(3-hydroxyphenyl)-prop-2-en-1-one

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The title molecule, $C_{15}H_{11}BrO_2$, is approximately planar and the dihedral angle between the two aromatic rings is 10.2 (2)°. The H atoms of the central enone moiety are *trans*. The molecules form centrosymmetric hydrogen-bonded dimers *via* intermolecular $O—H\cdots O$ hydrogen bonds ($H\cdots O$ = 2.02 Å and $O—H\cdots O$ = 172°).

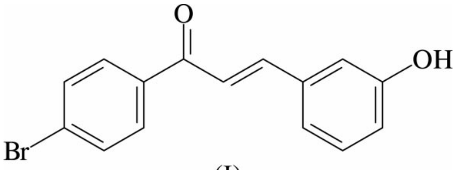
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.091
Data-to-parameter ratio = 15.5

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

Comment

Chalcones (1,3-diarylpropen-1-ones) and their heterocyclic analogues possess a number of biological attributes and some of these have been reviewed. The antibacterial, fungistatic and fungicidal properties of these compounds have been reviewed by Opletalova (2000) and Opletalova & Sedivy (1999). The cytotoxic, anticancer, chemopreventative, mutagenic, antimicrobial, antiviral, antiprotozoal and insecticidal activities and enzyme-inhibitory properties of a variety of chalcones have been reviewed by Dimmock *et al.* (1999). Chalcones and their analogues are used as potential therapeutic agents in diseases of the cardiovascular system (Opletalova *et al.*, 2003). In recent years, the synthesis of polymers having a photosensitive functional group has been an active field of research in polymer science. Monomers having structures similar to that of the title compound, (I), have been polymerized in solution using free radical initiators (Balaji & Nanjundan, 2001; Subramanian *et al.*, 2001). These polymers undergo cross-linking upon irradiation with UV light or an electron beam and are used as photoresistors (Hyder Ali & Srinivasan, 1997; Rehab & Salahuddin, 1999). These photosensitive polymers find application in the fields of integrated circuit technology and photocurable coatings (Nagamatzu & Inui, 1977). More recently, it has been noted that bromo-substituted derivatives of chalcones frequently crystallize in non-centrosymmetric space groups, which is a criterion for second-order non-linear optic (NLO) properties (Zhao *et al.*, 2000). Against this background, and in order to obtain detailed information on its crystal structure, an X-ray study of (I) has been carried out.



(I)

Compound (I), a bromo-substituted chalcone, is found to crystallize in a centrosymmetric space group and therefore has no second-order NLO properties. The molecule of (I) (Fig. 1) is approximately planar. The enone moiety of the molecule containing atoms C7, C8, C9 and O1 is planar to within

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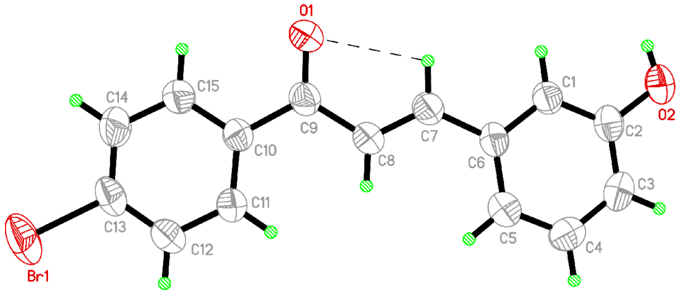

Figure 1
The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

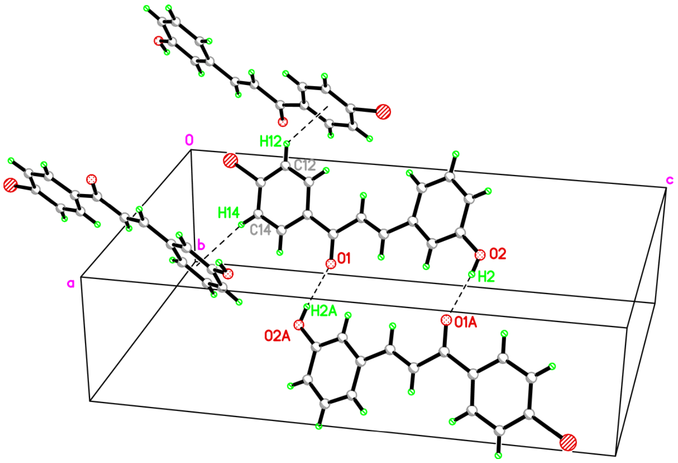

Figure 2
Part of the network structure of (I), showing O—H···O hydrogen-bonded dimers and C—H···π interactions (dashed lines). Only the atoms involved in the interactions are labelled. Atoms with a suffix A are generated by the symmetry operation $(1 - x, 1 - y, 1 - z)$.

±0.023 (2) Å. The least-squares plane through the enone moiety makes dihedral angles of 7.8 (2) and 3.9 (2)°, respectively, with the C1–C6 and C10–C15 benzene rings. The dihedral angle between the benzene rings is 10.2 (2)°. The H atoms attached to atoms C7 and C8 are *trans* to each other. The lengths of the C6—C7 [1.458 (3) Å], C7═C8 [1.316 (3) Å], C8—C9 [1.467 (4) Å], C9—C10 [1.492 (3) Å] and C9═O1 [1.223 (3) Å] bonds indicate conjugation. As observed in similar structures (Ravishankar, Chinnakali, Nanjundan, Jone Selvamalar *et al.*, 2003; Ravishankar, Chinnakali, Nanjundan, Radhakrishnan *et al.*, 2003), the strain induced by the short H5···H8 [2.28 Å] contact causes the bond angles C5—C6—C7 [123.1 (2)°] and C6—C7—C8 [128.6 (3)°] to deviate significantly from 120°. Also, the short H8···H11 [2.08 Å] contact results in a slight widening of the C9—C10—C11 angle to 123.4 (2)°. The weak intramolecular C7—H7···O1 interaction generates an *S*(5) ring motif.

In the crystal structure of (I), inversion-related molecules at (x, y, z) and $(1 - x, 1 - y, 1 - z)$ are linked by O2—H2···O1 hydrogen bonds into cyclic centrosymmetric $R_2^2(18)$ dimers (Table 1). The dimers are interlinked by weak C—H···π interactions involving both aromatic rings leading to the formation of a three-dimensional network (Fig. 2). A short Br···Br$(-x, -y, -z)$ contact of 3.5763 (5) Å is also observed in the structure.

Experimental

Compound (I) was obtained by the Claisen–Schmidt condensation of 4-bromoacetophenone (3.96 g, 0.02 mol) and 3-hydroxybenzaldehyde (2.46 g, 0.02 mol) in ethanol in the presence of aqueous NaOH. The product was isolated by neutralizing the reaction mixture with dilute hydrochloric acid. The crude product was recrystallized from ethanol.

Crystal data

$C_{15}H_{11}BrO_2$
$M_r = 303.15$
Monoclinic, $P2_1/c$
$a = 11.7495$ (13) Å
$b = 5.4876$ (6) Å
$c = 20.165$ (2) Å
$\beta = 95.918$ (2)°
$V = 1293.2$ (2) Å^3
$Z = 4$
$D_x = 1.557$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2004 reflections
$\theta = 2.5$–27.6°
$\mu = 3.17$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.23 × 0.16 × 0.12 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.514$, $T_{\max} = 0.686$
6678 measured reflections
2538 independent reflections
1905 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\max} = 26.0°$
$h = -14 \rightarrow 14$
$k = -4 \rightarrow 6$
$l = -24 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.091$
$S = 1.02$
2538 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.6438P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.45$ e Å^{-3}
$\Delta\rho_{\min} = -0.46$ e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring and *Cg*2 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1$^{\rm i}$	0.82	2.02	2.837 (3)	172
C7—H7···O1	0.93	2.43	2.782 (3)	102
C12—H12···*Cg*2$^{\rm ii}$	0.93	2.78	3.482 (4)	132
C14—H14···*Cg*1$^{\rm iii}$	0.93	3.02	3.590 (3)	121

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

H atoms were placed in calculated positions, with O—H and C—H distances of 0.82 and 0.93 Å, respectively. The $U_{\rm iso}$(H) values were constrained to be 1.5$U_{\rm eq}$ of the carrier atom for hydroxyl H and 1.2$U_{\rm eq}$ for the remaining H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement and data reduction: *SAINT* (Siemens, 1996); program(s) used to solve and refine structure: *SHELXTL* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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