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1-(4-Bromophenyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.129
Data-to-parameter ratio = 27.5

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

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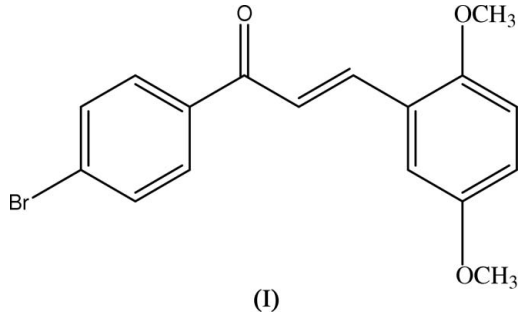
In the title compound, $C_{17}H_{15}BrO_3$, the dihedral angle between the benzene rings is 18.34 (13)°. The crystal structure is stabilized by intermolecular C—H···O interactions and Br···O short contacts.

Comment

Chalcones display a wide variety of pharmacological properties, including antibacterial, antiviral, antimutagenic, antimitotic, anti-inflammatory, anti-ulcerative and hepatoprotective activities (Batt *et al.*, 1993; Sogawa *et al.*, 1994; Arty *et al.*, 2000). In addition, with appropriate subtituents, chalcones are a class of non-linear optical materials (Fichou *et al.*, 1988; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006). In these materials, the C═O bond acts as the electron-withdrawing group, and electron-rich subtituents on the aromatic rings serve as the electron–donating group, forming a so-called $D—\pi\cdots A$ type molecule. During our search for chalcone non-linear optical materials, the title compound (I), was synthesized. We present here a study of molecular packing in the title compound, (I), which crystallizes in a centrosymmetric crystal structure and hence has no second-order NLO properties.



(I)

The bond lengths and angles for (I) are within normal ranges (Allen *et al.*, 1987) and are comparable to those in related structures (Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Santhi & Fun, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Selvam *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Ravishankar *et al.*, 2005; Teh *et al.*, 2006; Ng *et al.*, 2006; Patil *et al.*, 2006). The dihedral angle between the benzene rings is 18.34 (13)°. The enone group makes dihedral angles of 16.62 (10) and 1.8 (1)° with the C1–C6 and C10–C15 rings, respectively. The two methoxy groups attached at C11 and C14 are almost coplanar with the benzene ring, with C16—O3—C14—C13 and C17—O2—C11—C12 torsion angles of 2.8 (4) and 10.8 (4)°, respectively.

An intramolecular C—H···O hydrogen bond is observed in (I) (Table 1 and Fig. 1). The molecules form chains in the *ac* plane through C—H···O intermolecular hydrogen bonds and Br1···O3($\frac{1}{2}-x,\frac{3}{2}-y,-z$) [3.187 (2) Å] short contacts. These chains are stacked along the *b* axis, forming layers (Fig. 2).

Experimental

Compound (I) was obtained by the condensation of 2,5-dimethoxybenzaldehyde (0.01 mol) with 4-bromoacetophenone (0.01 mol) in ethanol (60 ml) in the presence of a catalytic amount of NaOH (5 ml, 20%). After stirring strongly for 2 h, the contents of the flask were poured into ice-cold water, and the resulting crude solid was collected by filtration. The compound was dried and purified by recrystallization from actone. The purity of the compound was checked by thin layer chromatography. Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of an acetone solution at room temperature, over a period of 10 d.

Crystal data

$C_{17}H_{15}BrO_3$
$M_r = 347.20$
Monoclinic, $C2/c$
$a = 34.1239\ (8)$ Å
$b = 4.6292\ (1)$ Å
$c = 19.0194\ (4)$ Å
$\beta = 103.001\ (2)^\circ$
$V = 2927.41\ (11)$ Å^3
$Z = 8$
$D_x = 1.576$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8581 reflections
$\theta = 1.2$–32.5°
$\mu = 2.82$ mm^{-1}
$T = 100.0\ (1)$ K
Block, yellow
0.22 × 0.16 × 0.16 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.474$, $T_{max} = 0.655$
46788 measured reflections
5274 independent reflections
3716 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 32.5^\circ$
$h = -48 \rightarrow 51$
$k = -6 \rightarrow 6$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.129$
$S = 1.16$
5274 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2 + 2.8596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -1.01$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O2	0.93	2.39	2.746 (3)	103
C17—H17A···O1^{i}	0.96	2.53	3.088 (4)	118

Symmetry code: (i) $-x+1, y+1, -z+\frac{1}{2}$.

H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.96 Å. The U_{iso}(H) values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. The highest peak is located 0.66 Å from atom O1 and the deepest hole is 0.78 Å from Br1.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

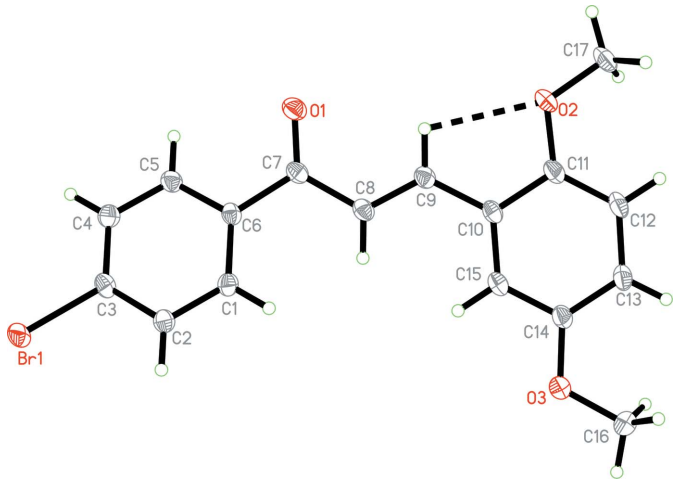


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates an intramolecular hydrogen bond.

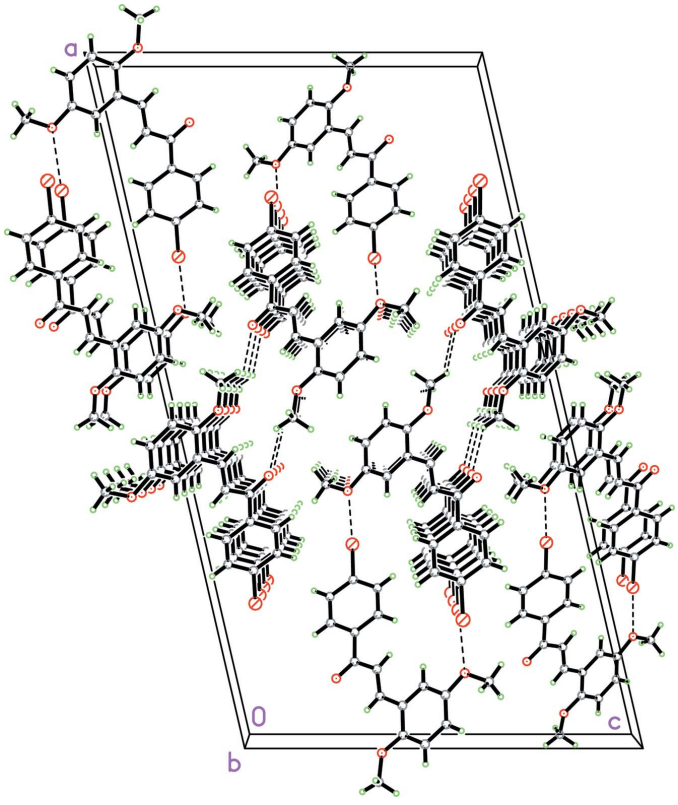


Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds and close Br···O contacts are shown as dashed lines.

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