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Key indicators

Single-crystal X-ray study
T = 173 K
Mean $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$
R factor = 0.067
wR factor = 0.181
Data-to-parameter ratio = 14.2

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

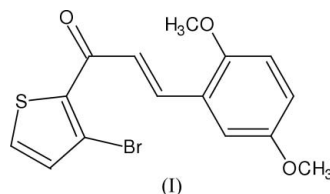
(2E)-1-(3-Bromo-2-thienyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one

The molecules of the title compound, $\text{C}_{15}\text{H}_{13}\text{BrO}_3\text{S}$, are almost planar and do not show unusual geometric parameters. The crystal packing is characterized by short $\text{C}-\text{H}\cdots\text{O}$ contacts.

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Comment

Chalcones and their heterocyclic analogues show numerous biological effects (Opletalova & Sedivy, 1999; Dimmock *et al.*, 1999). In addition, with appropriate substituents, chalcones are a class of non-linear optical (NLO) materials (Fichou *et al.*, 1988; Butcher *et al.*, 2006; Harrison *et al.*, 2006).



The crystal structures of 3-hydroxy-1,3-bis(2-thienyl)prop-2-en-1-one (Baxter *et al.*, 1990) and 1-(4-chlorophenyl)-3-(2-thienyl)prop-2-en-1-one (Ng *et al.*, 2006) have been reported. In continuation of our work on the crystal structures of chalcones (Yathirajan *et al.*, 2006a,b), the present paper reports the crystal structure of the title compound, (I), (Fig. 1).

The bond lengths and angles in (I) can be regarded as normal (Cambridge Structural Database, Version 5.27; Allen, 2002) and all the non-H atoms are close to coplanar (r.m.s. deviation = 0.130 Å). The molecular structure and the crystal packing of (I) are characterized by short $\text{C}-\text{H}\cdots\text{O}$ contacts (Table 1).

Experimental

2-Acetyl-3-bromothiophene (10 g, 0.048 mol) in methanol (50 ml) was mixed with 2,5-dimethoxybenzaldehyde (8 g, 0.048 mol) and the mixture was treated with 10 ml of 30% potassium hydroxide solution at 278 K. The reaction mixture was then brought to room temperature and stirred for 4 h. The precipitated solid was filtered and washed with water, dried and recrystallized from acetone to yield crystals of (I) (yield: 83%; m.p.: 375–377 K). Analysis for $\text{C}_{15}\text{H}_{13}\text{BrO}_3\text{S}$: found (calculated); C: 50.93 (51.00%); H: 3.63 (3.71%).

Crystal data

$\text{C}_{15}\text{H}_{13}\text{BrO}_3\text{S}$	$Z = 2$
$M_r = 353.22$	$D_x = 1.624 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 5.2240 (5) \text{ \AA}$	$\mu = 2.99 \text{ mm}^{-1}$
$b = 9.3265 (14) \text{ \AA}$	$T = 173 (2) \text{ K}$
$c = 14.8968 (16) \text{ \AA}$	Block, yellow
$\beta = 95.622 (9)^\circ$	$0.36 \times 0.33 \times 0.32 \text{ mm}$
$V = 722.31 (15) \text{ \AA}^3$	

Data collection

STOE IPDS II two-circle diffractometer
 ω scans
 Absorption correction: multi-scan *MULABS* (Spek, 2003; Blessing, 1995)
 $T_{\min} = 0.362$, $T_{\max} = 0.398$

4264 measured reflections
 2604 independent reflections
 2465 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$
 $\theta_{\text{max}} = 27.1^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.181$
 $S = 1.06$
 2604 reflections
 183 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1481P)^2 + 0.1692P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 1.14 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.75 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack (1983),
 926 Friedel pairs
 Flack parameter: 0.025 (18)

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C4-H4\cdots O5^i$	0.95	2.37	3.296 (8)	164
$C17-H17B\cdots O5^{ii}$	0.98	2.41	3.331 (9)	157
$C7-H7\cdots O5$	0.95	2.47	2.798 (8)	100
$C7-H7\cdots O17$	0.95	2.41	2.763 (8)	102

Symmetry codes: (i) $-x + 3, y + \frac{1}{2}, -z + 2$; (ii) $-x + 1, y - \frac{1}{2}, -z + 2$.

The H atoms were found in a difference map and then placed in idealized positions ($C-H = 0.95-0.98 \text{ \AA}$) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The methyl groups were allowed to rotate but not to tip to best fit the electron density. The highest peak in the final difference map is located 0.79 \AA from atom Br1 and the deepest hole 0.82 \AA from Br1.

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*.

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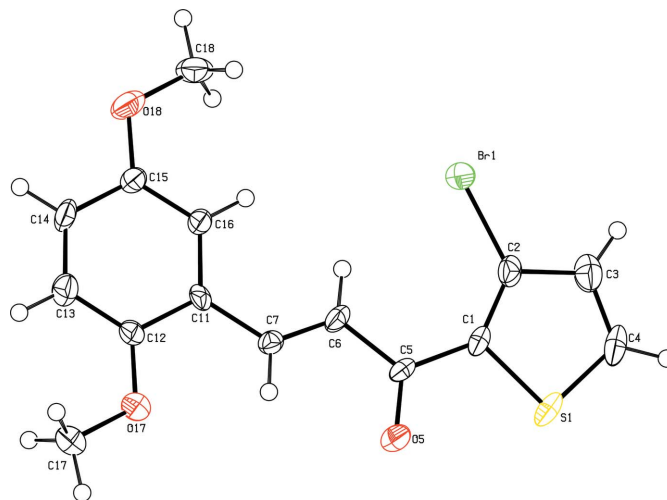


Figure 1

View of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

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