

## 1-Phenyl-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one

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## Key indicators

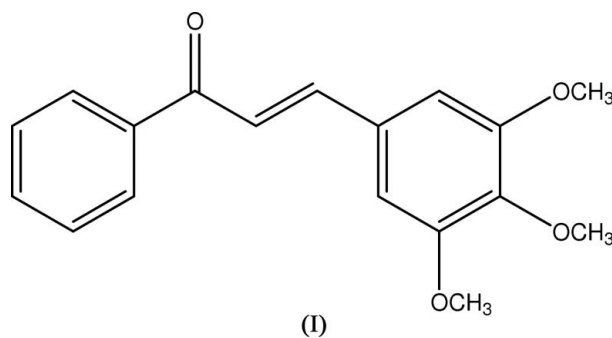
Single-crystal X-ray study  
 $T = 120$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.091  
Data-to-parameter ratio = 13.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{18}\text{H}_{18}\text{O}_4$ , the dihedral angle between the benzene rings is  $9.07$  ( $7$ )°. Intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions form chains along the  $c$  axis. The crystal structure is further stabilized by  $\text{C}-\text{H}\cdots\pi$  interactions.

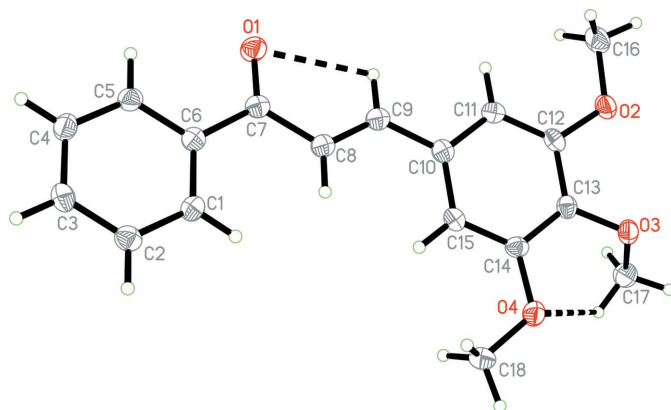
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## Comment

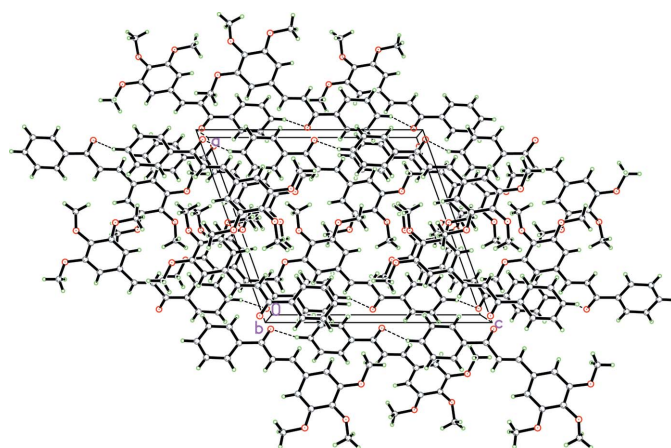
Chalcones, particularly a series of dimethoxy- and trimethoxychalcone derivatives, with various patterns of fluorination, are important compounds for their influence on nitric oxide production in lipopolysaccharide-stimulated murine RAW 264.7 cells (Rojas *et al.*, 2002). They are also potential new cancer chemopreventive agents (Bertl *et al.*, 2004). Recently, it has been noted that, among many organic compounds reported for their second harmonic generation, chalcone derivatives have excellent blue light transmittance and good crystallizability (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Zhao *et al.*, 2000). Against this background, and in order to obtain detailed information on its crystal structure, a single-crystal X-ray study of the title compound, (I), has been carried out.



A molecular view of (I) is shown in Fig. 1. Bond lengths and angles have normal values (Allen *et al.*, 1987) and are comparable with those observed for 1-(4-aminophenyl)-3-(3-bromophenyl)prop-2-en-1-one (Sathiya Moorthi, Chinnakali, Nanjundan, Santhi *et al.*, 2005), 1-(4-bromophenyl)-3-(3-hydroxyphenyl)prop-2-en-1-one (Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005), 1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005), 1-(4-chlorophenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one (Ravishankar *et al.*, 2005), 3-(3-bromophenyl)-1-phenylprop-2-en-1-one (Ng *et al.*, 2006) and 3-(4-methoxyphenyl)-1-(4-nitrophenyl)prop-2-en-1-one (Patil *et al.*, 2006). The least-squares plane through the enone fragment makes dihedral angles of  $1.89$  ( $10$ ) and  $8.42$  ( $8$ )° with the C1–C6 and C10–C15 benzene rings,



**Figure 1**  
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen bonds are shown as dashed lines.



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

respectively. The dihedral angle between the benzene rings is  $9.07(7)^\circ$ . The two methoxy groups attached at C12 and C14 are almost coplanar with the C10–C15 benzene ring while the third methoxy group attached at C13 is twisted away from it with a C17–O3–C13–C14 torsion angle of  $71.41(16)^\circ$ .

Two intramolecular C–H $\cdots$ O hydrogen bonds are observed in the molecular structure (Table 1). The intramolecular C9–H9 $\cdots$ O1 interaction generates an *S*(5) ring motif (Bernstein *et al.*, 1995). The crystal structure is stabilized by C–H $\cdots$ O interactions (Table 1) which form chains along the *c* axis. The crystal structure is further stabilized by C–H $\cdots$  $\pi$  interactions (Table 1) involving the C10–C15 ring.

## Experimental

Compound (I) was obtained by the Claisen–Schmidt condensation of acetophenone (0.02 mol, 2.342 ml) and 3,4,5-trimethoxybenzaldehyde (0.02 mol, 3.924 g) in ethanol (40 ml) in the presence of aqueous NaOH (20%, 10 ml). The mixture was stirred for 2 h and allowed to stand for 24 h. The resulting solid mass was collected by filtration, washed with ice-cold water and dried. The compound was recrystallized twice from acetone. Crystals of (I) suitable for X-ray diffraction were obtained in 7 d by the slow evaporation technique, using acetone as the solvent.

## Crystal data

C<sub>18</sub>H<sub>18</sub>O<sub>4</sub>  
*M<sub>r</sub>* = 298.32  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 13.5136 (4) Å  
*b* = 7.8414 (3) Å  
*c* = 14.9854 (5) Å  
 $\beta$  = 109.823 (2) $^\circ$   
*V* = 1493.84 (9) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.326 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation  
 Cell parameters from 5611 reflections  
 $\theta$  = 2.8–25.0 $^\circ$   
 $\mu$  = 0.09 mm<sup>-1</sup>  
*T* = 120.0 (1) K  
 Rhombohedron, yellow  
 0.68 × 0.66 × 0.48 mm

## Data collection

Brucker SMART APEX2 CCD  
 area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2005)  
*T<sub>min</sub>* = 0.862, *T<sub>max</sub>* = 0.957  
 13327 measured reflections

2632 independent reflections  
 2394 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.021  
 $\theta_{\max}$  = 25.0 $^\circ$   
*h* = -16 → 16  
*k* = -9 → 9  
*l* = -17 → 17

## Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.037  
*wR*(*F*<sup>2</sup>) = 0.091  
*S* = 1.03  
 2632 reflections  
 203 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 1.0117P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.65 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.25 \text{ e } \text{Å}^{-3}$   
 Extinction correction: *SHELXTL*  
 Extinction coefficient: 0.0095 (13)

**Table 1**

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

<i>D</i> –H $\cdots$ <i>A</i>	<i>D</i> –H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> –H $\cdots$ <i>A</i>
C3–H3 $\cdots$ O1 <sup>i</sup>	0.95	2.56	3.248 (2)	129
C9–H9 $\cdots$ O1	0.95	2.46	2.805 (2)	101
C17–H17C $\cdots$ O4	0.98	2.37	2.966 (2)	118
C2–H2 $\cdots$ Cg <sup>ii</sup>	0.95	2.76	3.500 (2)	135

Symmetry codes: (i) *x*,  $-y + \frac{1}{2}$ , *z* +  $\frac{1}{2}$ ; (ii) *x*,  $-y + \frac{3}{2}$ , *z* +  $\frac{1}{2}$ . Cg is the centroid of the C10–C15 ring.

H atoms were placed in calculated positions, with C–H distances in the range 0.95–0.98 Å. The *U*<sub>iso</sub>(H) values were constrained to be 1.5*U*<sub>eq</sub> of the carrier atom for methyl H atoms and 1.2*U*<sub>eq</sub> for the remaining H atoms.

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).

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