

(E)-3-[4-(Decyloxy)phenyl]-1-(4-hydroxyphenyl)prop-2-en-1-one

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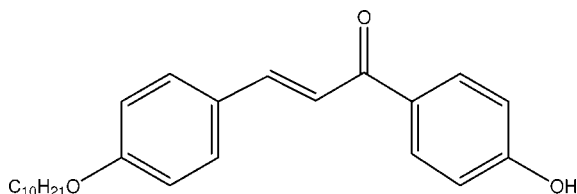
Received 15 April 2009; accepted 17 April 2009

Key indicators: single-crystal X-ray study; *T* = 100 K; mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$ ; *R* factor = 0.064; *wR* factor = 0.132; data-to-parameter ratio = 19.1.

In the title compound,  $\text{C}_{25}\text{H}_{32}\text{O}_3$ , the enone group adopts an *s-cis* conformation. The alkoxy unit is nearly planar and is in a *trans* conformation. The two benzene rings make a dihedral angle of  $18.87(9)^\circ$ . In the crystal structure, molecules are linked into chains running along the *a* axis by intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds involving the hydroxy and keto groups. The chains are crosslinked along the *b* axis via  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, forming a two-dimensional network parallel to the *ab* plane.

Related literature

For the biological properties of chalcone derivatives, see: Bhat *et al.* (2005); Xue *et al.* (2004); Satyanarayana *et al.* (2004); Lee *et al.* (2006). For related structures, see: Ng *et al.* (2006); Razak *et al.* (2009); Ngaini, Fadzillah *et al.* (2009); Ngaini, Rahman *et al.* (2009). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



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Experimental

Crystal data

$\text{C}_{25}\text{H}_{32}\text{O}_3$   
 $M_r = 380.51$   
 Orthorhombic, *Pbca*  
 $a = 10.5192(3) \text{ \AA}$   
 $b = 9.9839(3) \text{ \AA}$   
 $c = 40.8415(12) \text{ \AA}$   
 $V = 4289.3(2) \text{ \AA}^3$   
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.08 \text{ mm}^{-1}$   
 $T = 100 \text{ K}$   
 $0.58 \times 0.49 \times 0.03 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2005)  
 $T_{\text{min}} = 0.957, T_{\text{max}} = 0.998$   
 42832 measured reflections  
 4922 independent reflections  
 3526 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.082$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$   
 $wR(F^2) = 0.132$   
 $S = 1.10$   
 4922 reflections  
 258 parameters  
 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

Table 1

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

<i>D</i> — <i>H</i> ··· <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> — <i>H</i> ··· <i>A</i>
$\text{O1}-\text{H1O1}\cdots\text{O2}^{\text{i}}$	0.95 (3)	1.71 (3)	2.655 (2)	177 (3)
$\text{C5}-\text{H5}\cdots\text{O1}^{\text{ii}}$	0.93	2.48	3.340 (2)	155

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and IAR thank the Malaysian government and Universiti Sains Malaysia for Science Fund grant No. 305/PFIZIK/613312 and for Research University Golden Goose grant No. 1001/PFIZIK/811012. ZN and HH thank Universiti Malaysia Sarawak for Geran Penyelidikan Dana Khas Inovasi grant No. DI/01/2007(01). NIAR thanks the Malaysian government and Universiti Malaysia Sarawak for providing a scholarship for postgraduate studies.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2782).

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