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(E)-3-(4-Decyloxyphenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one

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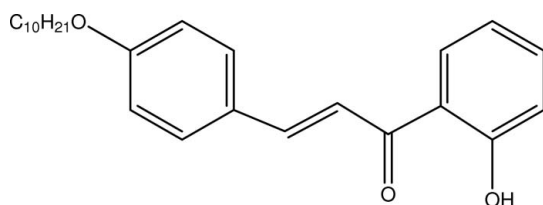
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.058; wR factor = 0.165; data-to-parameter ratio = 24.1.

In the title compound, $\text{C}_{25}\text{H}_{32}\text{O}_3$, the enone group is in an *s-cis* configuration. The dihedral angle between the benzene rings is $8.84(7)^\circ$. An intramolecular $\text{O}-\text{H}\cdots\text{O}$ interaction between the keto and hydroxy groups forms an $S(6)$ ring motif. Intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions link the molecules into supramolecular chains along the c axis which are subsequently stacked down the b axis; the crystal structure is further consolidated by $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For general background, see: Bhat *et al.* (2005); Xue *et al.* (2004); Satyanarayana *et al.* (2004); Won *et al.* (2005); Zhao *et al.* (2005). For related structures, see: Ng, Razak *et al.* (2006); Ng, Patil *et al.* (2006); Razak *et al.* (2009); Ngaini *et al.* (2009). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer, 1986.



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Experimental

Crystal data

$\text{C}_{25}\text{H}_{32}\text{O}_3$
 $M_r = 380.51$
 Monoclinic, $P2_1/c$
 $a = 21.2700(4)$ Å
 $b = 7.6779(2)$ Å
 $c = 13.2330(3)$ Å
 $\beta = 101.720(1)^\circ$
 $V = 2116.01(8)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 100$ K
 $0.44 \times 0.28 \times 0.04$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.967$, $T_{\max} = 0.997$
 25687 measured reflections
 6221 independent reflections
 4014 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.165$
 $S = 1.04$
 6221 reflections
 258 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.37$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1O1}\cdots\text{O2}$	0.91 (2)	1.68 (2)	2.526 (2)	152 (2)
$\text{C15}-\text{H15A}\cdots\text{O3}^{\text{i}}$	0.93	2.48	3.406 (2)	174
$\text{C20}-\text{H20B}\cdots\text{Cg1}^{\text{ii}}$	0.97	2.85	3.702 (2)	147
$\text{C22}-\text{H22A}\cdots\text{Cg1}^{\text{iii}}$	0.97	2.84	3.712 (2)	149
$\text{C16}-\text{H16A}\cdots\text{Cg2}^{\text{iii}}$	0.97	2.87	3.596 (2)	132

Symmetry codes: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + 1, -y, -z + 1$; (iii) $-x + 1, -y + 1, -z + 1$. Cg1 and Cg2 are the centroids of the C1-C6 and C10-C15 rings, respectively.

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2402).

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