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

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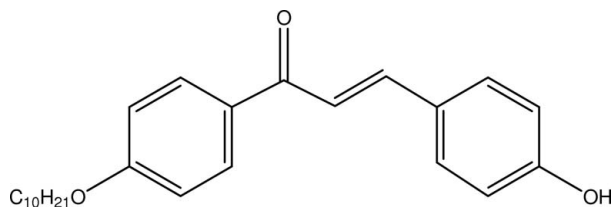
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.056; wR factor = 0.153; data-to-parameter ratio = 32.9.

In the title compound, $\text{C}_{25}\text{H}_{32}\text{O}_3$, the asymmetric unit contains two crystallographically independent molecules: both enone groups adopt an *s-cis* configuration. In the crystal, $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ intermolecular interactions form bifurcated hydrogen bonds, which generate $R_2^1(6)$ ring motifs. These intermolecular interactions link the molecules into one-dimensional chains along the $[10\bar{1}]$ direction. The crystal structure is further stabilized by $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For general background to the biological properties of chalcone derivatives, see: Bhat *et al.* (2005); Xue *et al.* (2004); Satyanarayana *et al.* (2004); Zhao *et al.* (2005); Yayli *et al.* (2006). For related structures, see: Ng, Razak *et al.* (2006); Ng, Patil *et al.* (2006). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$\text{C}_{25}\text{H}_{32}\text{O}_3$
 $M_r = 380.51$
 Monoclinic, $P2_1/c$
 $a = 12.4437$ (2) Å
 $b = 35.5191$ (6) Å
 $c = 9.8004$ (2) Å
 $\beta = 99.284$ (1)°
 $V = 4274.93$ (13) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 100$ K
 $0.52 \times 0.44 \times 0.35$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.962$, $T_{\max} = 0.974$
 62626 measured reflections
 16928 independent reflections
 12634 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.153$
 $S = 1.04$
 16928 reflections
 515 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.54$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{O1A}-\text{H1OA}\cdots\text{O2B}^i$ | 0.91 (2) | 1.80 (2) | 2.711 (1) | 179 (3) |
| $\text{O1B}-\text{H1OB}\cdots\text{O2A}^{ii}$ | 0.91 (2) | 1.81 (2) | 2.716 (1) | 176 (2) |
| $\text{C4A}-\text{H4AA}\cdots\text{O2B}^i$ | 0.93 | 2.50 | 3.185 (1) | 131 |
| $\text{C4B}-\text{H4BA}\cdots\text{O2A}^{ii}$ | 0.93 | 2.50 | 3.192 (1) | 131 |
| $\text{C14B}-\text{H14B}\cdots\text{O3A}$ | 0.93 | 2.56 | 3.485 (1) | 173 |
| $\text{C18B}-\text{H18C}\cdots\text{Cg1}^{iii}$ | 0.97 | 2.85 | 3.696 (1) | 146 |
| $\text{C24B}-\text{H24D}\cdots\text{Cg2}^{iii}$ | 0.97 | 2.71 | 3.554 (1) | 145 |
| $\text{C22A}-\text{H22B}\cdots\text{Cg3}^{iv}$ | 0.97 | 2.95 | 3.743 (1) | 140 |

Symmetry codes: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (ii) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 1, -y, -z + 2$; (iv) $x, -y - \frac{1}{2}, z - \frac{3}{2}$. Cg1, Cg2 and Cg3 are the centroids of the C1A-C6A, C10B-C15B and C1B-C6B 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: AT2746).

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