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

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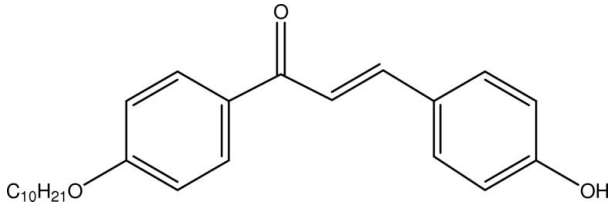
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.056; wR factor = 0.153; data-to-parameter ratio = 32.9.

In the title compound, $C_{25}H_{32}O_3$, the asymmetric unit contains two crystallographically independent molecules: both enone groups adopt an *s-cis* configuration. In the crystal, O—H···O and C—H···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 C—H···π 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

$C_{25}H_{32}O_3$
M_r = 380.51
Monoclinic, $P2_1/c$
a = 12.4437 (2) Å
b = 35.5191 (6) Å
c = 9.8004 (2) Å
β = 99.284 (1)°
V = 4274.93 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.52 × 0.44 × 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_{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
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

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