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

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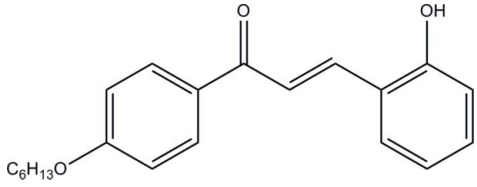
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.133; data-to-parameter ratio = 20.6.

In the title compound, $C_{21}H_{24}O_3$, the enone moiety adopts an *s-cis* conformation and the dihedral angle between the benzene rings is 12.89 (6)°. The hexyloxy tail adopts an extended conformation. In the crystal, inversion dimers are linked by pairs of O—H···O hydrogen bonds and pairs of C—H···O interactions, forming two $R_2^2(7)$ and one $R_2^2(10)$ loops. The dimers are then arranged into sheets lying parallel to (201) and weak C—H···π interactions consolidate the packing.

Related literature

For a related structure and background to the biological properties of chalcones, see: Ngaini *et al.* (2011). For related structures, see: Razak *et al.* (2009); Ngaini *et al.* (2010). For graph-set theory, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{21}H_{24}O_3$
M_r = 324.40
Triclinic, $P\overline{1}$
a = 7.485 (2) Å
b = 10.834 (3) Å
c = 11.673 (3) Å
α = 73.858 (5)°
β = 77.961 (6)°
γ = 76.941 (6)°
V = 874.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.47 × 0.14 × 0.12 mm

Data collection

Bruker APEX DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.963, T_{max} = 0.991
17565 measured reflections
4576 independent reflections
3781 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.133
S = 1.02
4576 reflections
222 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1*O2*···O1^{i}	0.94 (2)	1.78 (2)	2.6862 (15)	163.3 (19)
C7—H7*A*···O2^{i}	0.93	2.37	3.2526 (18)	158
C16—H16*A*···*Cg*1^{ii}	0.97	2.91	3.6117 (16)	130

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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: HB6948).

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