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

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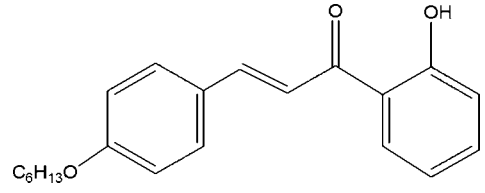
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.070; wR factor = 0.190; data-to-parameter ratio = 22.6.

In the title compound, $C_{21}H_{24}O_3$, the conformation of the enone group is *s–cis*. The benzene rings are inclined at an angle of 7.9 (1)°. The alkoxy tail is planar, with a maximum deviation from the least-squares plane of 0.009 (2) Å, and adopts a *trans* conformation throughout. An intramolecular O—H···O interaction between the keto and hydroxy groups forms S(6) ring motifs. In the crystal, molecules are arranged in a head-to-tail manner down the *a* axis and are subsequently stacked along the *b* axis, forming molecular sheets parallel to the *ab* plane. The crystal structure is further stabilized by weak C—H···π interactions and short C···O [3.376 (2) Å] contacts.

Related literature

For the biological properties of chalcone derivatives, see: Bhat *et al.* (2005); Xue *et al.* (2004); Zhao *et al.* (2005); Lee *et al.* (2006). For related structures, see: Razak, Fun, Ngaini, Rahman & Hussain (2009); Razak, Fun, Ngaini, Fadzillah & Hussain (2009*a*,*b*); Ngaini, Fadzillah *et al.* (2009); Ngaini, Rahman *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

$C_{21}H_{24}O_3$
M_r = 324.40
Monoclinic, $P2_1/c$
a = 19.6443 (5) Å
b = 7.1966 (2) Å
c = 12.6520 (3) Å
β = 106.438 (2)°
V = 1715.53 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.47 × 0.12 × 0.04 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.962, T_{max} = 0.997
20873 measured reflections
5025 independent reflections
2783 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.190
S = 1.05
5025 reflections
222 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*1···O2	0.90 (3)	1.68 (3)	2.507 (2)	152 (2)
C20—H20*A*···*Cg*1^{i}	0.97	2.84	3.657 (2)	142
C20—H20*B*···*Cg*1^{ii}	0.97	2.78	3.637 (2)	147

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$. *Cg*1 is the centroid of the C1-C6 ring.

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: SJ2623).

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