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

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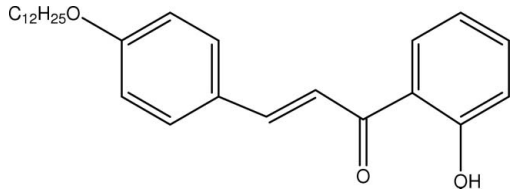
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.069; wR factor = 0.206; data-to-parameter ratio = 15.7.

In the title compound, $C_{27}H_{36}O_3$, the asymmetric unit consists of two crystallographically independent molecules. The aromatic rings form dihedral angles of 17.1 (2) and 17.6 (2)° in the two molecules. In both molecules, the enone groups adopt an *s–cis* conformation and the alkoxyl chains are in *trans* conformations curving out of the zigzag plane. Intramolecular O—H···O hydrogen bonds involving the keto and hydroxy groups generate S(6) ring motifs. The molecules are stacked alternately in a head-to-tail fashion along the *a* axis and the crystal structure is stabilized by weak C—H···π interactions. The crystal studied was a non-merohedral twin, the ratio of components being 0.788 (2):0.212 (2).

Related literature

For general background to the biological activity of chalcone derivatives, see: Bhat *et al.* (2005); Xue *et al.* (2004); Satyanarayana *et al.* (2004); Zhao *et al.* (2005); Lee *et al.* (2006). For related structures, see: Ng *et al.* (2006); Razak *et al.* (2009); Ngaini, Fadzillah *et al.* (2009); Ngaini, Rahman *et al.* (2009). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{27}H_{36}O_3$
M_r = 408.56
Triclinic, $P\overline{1}$
a = 7.4953 (6) Å
b = 13.4714 (9) Å
c = 23.7874 (18) Å
α = 75.116 (4)°
β = 83.876 (5)°
γ = 84.669 (5)°
V = 2302.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.55 × 0.13 × 0.06 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.960, T_{max} = 0.996
8571 measured reflections
8571 independent reflections
4737 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.206
S = 1.03
8571 reflections
546 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*A*—H1*A*···O2*A*	0.82	1.79	2.513 (4)	146
O1*B*—H1*B*···O2*B*	0.82	1.81	2.530 (4)	146
C22*B*—H22*C*···*Cg*1^{i}	0.97	2.77	3.654 (4)	151
C17*B*—H17*D*···*Cg*2	0.97	2.82	3.612 (4)	139
C22*A*—H22*B*···*Cg*3	0.97	2.93	3.765 (4)	145

Symmetry code: (i) $x-1, y, z$. *Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1*A*--C6*A*, C10*A*–C15*A* and C1*B*–C6*B* rings, respectively.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2802).