(E)-1-(3-Hy-droxy-phen-yl)-3-[4-(tetra-dec-yl-oxy)phen-yl]prop-2-en-1-one

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(*E*)-1-(3-Hydroxyphenyl)-3-[4-(tetradecyloxy)phenyl]prop-2-en-1-one

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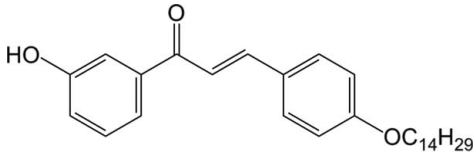
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.147; data-to-parameter ratio = 24.4.

In the title compound, $C_{29}H_{40}O_3$, the enone moiety adopts an *s-cis* conformation. The dihedral angle between the benzene rings is 4.33 (5)° The least-squares mean line through the tetradecyl side chain forms a dihedral angle of 83.99 (7)° with the normal to the attached benzene ring. In the crystal, O—H···O and C—H···O hydrogen bonds involving the keto and the hydroxy O atoms form ribbons along [$\bar{4}1\bar{1}$]. The crystal structure also features C—H···π interactions.

Related literature

For the biological properties of chalcone derivatives, see: Bhat *et al.* (2005); Xue *et al.* (2004); Won *et al.* (2005); Zhao *et al.* (2005); Satyanarayana *et al.* (2004). For related structures, see: Razak *et al.* (2009); Ngaini *et al.* (2010, 2011). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{29}H_{40}O_3$
M_r = 436.61
Triclinic, $P\bar{1}$
a = 6.5138 (16) Å
b = 10.155 (2) Å
c = 19.264 (5) Å
α = 75.361 (6)°
β = 85.872 (7)°
γ = 83.013 (6)°
V = 1222.6 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.29 × 0.12 × 0.08 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.979, T_{max} = 0.994
26295 measured reflections
7155 independent reflections
5052 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.147
S = 0.95
7155 reflections
293 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C10–C15 and C1–C6 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O1*···O2^{i}	0.93 (2)	1.80 (2)	2.7269 (14)	175.6 (18)
C29—H29*A*···O1^{ii}	0.96	2.44	3.3589 (18)	160
C17—H17*B*···*Cg*1^{iii}	0.97	2.73	3.6159 (16)	152
C28—H28*A*···*Cg*2^{iv}	0.97	2.93	3.8481 (16)	159

Symmetry codes: (i) $-x+3, -y, -z+1$; (ii) $x-4, y+1, z-1$; (iii) $x-1, y, z$; (iv) $x-3, y+1, z-1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); 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) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5001).

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