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(*E*)-1-(2,5-Dimethyl-3-thienyl)-3-(2-hydroxyphenyl)prop-2-en-1-one

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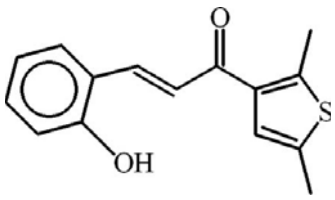
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.112; data-to-parameter ratio = 19.1.

In the title compound, $C_{15}H_{14}O_2S$, the dihedral angle between the aromatic rings is 8.46 –(8)°. The central enone group is planar (r.m.s. deviation = 0.0267 Å) and is oriented at a dihedral angle of 1.20 (9)° with respect to the benzene ring and at 8.27 (9)° with respect to the thiophene group. In the crystal, the molecules are linked into polymeric chains extending along the *b* axis due to intermolecular O—H···O hydrogen bonding. An *S*(6) ring motif is formed due to a short intramolecular C—H···O contact. C—H···π interactions involving a methyl group of the 2,5-dimethylthienyl group and the benzene ring are present. π–π interactions between the centroids of the benzene and heterocyclic rings [3.7691 (9) Å] also occur.

Related literature

For background to chalcones and their biological activity, see: Bandgar & Gawande (2010); Domínguez *et al.* (2001); Hans *et al.* (2010); Kayser & Kiderlen (2001); Mojzis *et al.* (2008); Vogel *et al.* (2010). For related structures, see: Asiri *et al.* (2010*a*,*b*); For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{15}H_{14}O_2S$
M_r = 258.32
Triclinic, $P\overline{1}$
a = 7.6095 (3) Å
b = 7.7900 (3) Å
c = 12.3109 (7) Å
α = 98.527 (2)°
β = 91.943 (2)°
γ = 115.551 (1)°
V = 647.19 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 K
0.30 × 0.24 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.968, T_{max} = 0.985
11156 measured reflections
3174 independent reflections
2720 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.112
S = 1.05
3174 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

*Cg*2 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.8900	2.7067 (14)	174
C8—H8···O1	0.93	2.2400	2.8416 (17)	122
C15—H15*A*···*Cg*2^{ii}	0.96	2.79	3.652 (2)	150

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2228).

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