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5-Phenyl-1-(2-thienyl)penta-2,4-dien-1-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.104
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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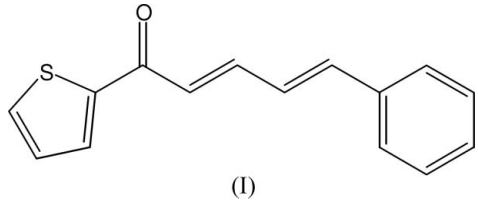
Both acyclic double bonds in the title molecule, $C_{15}H_{12}OS$, are *trans* configured. Geometric parameters are in the usual ranges.

Comment

α,β-Unsaturated ketones have been used as starting materials for the synthesis of various chemicals, including plastics, resins, pesticides, dyes and pharmaceuticals (Opdyke, 1973). The synthesis and biological evaluation of cyclopenta[*c*]thiophene-related compounds as new antitumour agents have been reported (Dallemagne *et al.*, 2002) and the title compound, (I), is a biologically active compound. Chalcones and pentadienones are found to exhibit non-linear optical activity (Uchida *et al.*, 1998). The crystal structure of 1,5-bis(4-chlorophenyl)penta-1,4-dien-3-one has been reported previously (Butcher *et al.*, 2006). In view of the importance of pentadienones, the crystal structure of compound (I) is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Allen *et al.*, 1987). Both acyclic double bonds are *trans* configured. The dihedral angle between the two aromatic rings is 4.68 (9)°. The central butadiene unit makes dihedral angles of 19.2 (1) and 16.8 (1)° with the thienyl group and the phenyl ring, respectively.

Experimental

The title compound was synthesized according to the method reported in the literature (Furniss *et al.*, 1989). The compound was

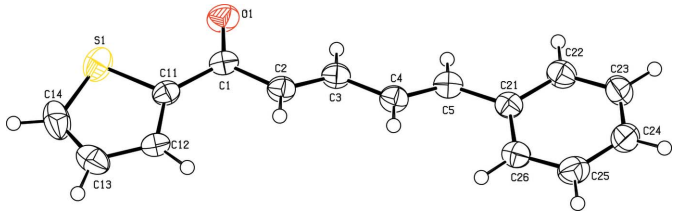


Figure 1
The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

purified by recrystallization from ethanol. Crystals were grown by slow evaporation of a solution of (I) in ethanol (yield 75%; m.p. 353–357 K). Analysis, found (calculated) for $C_{15}H_{12}OS$: C 74.20% (74.97%), H 5.08% (5.03%).

Crystal data

$C_{15}H_{12}OS$	$Z = 8$
$M_r = 240.31$	$D_x = 1.265$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 15.5571$ (12) Å	$\mu = 0.24$ mm^{-1}
$b = 10.2136$ (7) Å	$T = 173$ (2) K
$c = 15.8883$ (11) Å	Block, light yellow
$V = 2524.6$ (3) Å^3	0.42 × 0.35 × 0.22 mm

Data collection

Stoe IPDSII two-circle diffractometer	10971 measured reflections
	2353 independent reflections
ω scans	2080 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)	$R_{int} = 0.028$
	$\theta_{max} = 25.6^\circ$
$T_{min} = 0.909$, $T_{max} = 0.970$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.7828P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	
$wR(F^2) = 0.104$	
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
2353 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
H-atom parameters constrained	

H atoms were found in a difference map but they were refined using a riding model, with C—H = 0.95 Å for $C_{aromatic}$ and $C_{methylene}$, or 0.98 Å for methyl groups, and with $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C_{methyl})$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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