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3-(6-Methoxy-2-naphthyl)-1-(2-thienyl)-prop-2-en-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 = 0.037
wR factor = 0.102
Data-to-parameter ratio = 13.8

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

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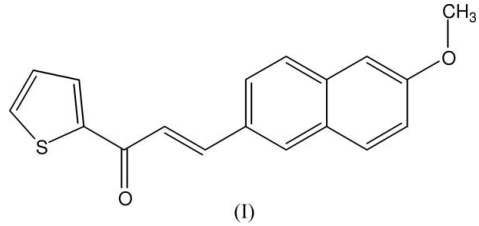
The molecule of the title compound, $C_{18}H_{14}O_2S$, is essentially planar. The central C=C double bond is *trans*-configured. Geometric parameters are in normal ranges.

Comment

The title compound, (I), is a biologically active compound. Chalcones and their heterocyclic analogues show various biological effects, *e.g.* anti-inflammatory, antitumour, antibacterial, antitubercular, antiviral, antiprotozoal, gastroprotective *etc.* (Opletalova & Sedivy, 1999). The cytotoxic, anticancer, antiviral, antiprotozoal and insecticidal activities of a variety of chalcones have been reviewed, as well as the enzyme-inhibitory properties and miscellaneous activities of some of these molecules (Dimmock *et al.*, 1999). In addition, with appropriate subsitutuents, chalcones are a class of nonlinear optical (NLO) materials (Fichou *et al.*, 1988; Goto *et al.*, 1991; Butcher *et al.*, 2006; Harrison *et al.*, 2006). The crystal structures of 3-hydroxy-1,3-bis(2-thienyl)prop-2-en-1-one (Baxter *et al.*, 1990), 1,3-bis(4-chlorophenyl)prop-2-en-1-one (Wang *et al.*, 2005), 1-(4-bromophenyl)-3-(2-thienyl)prop-2-en-1-one (Patil *et al.*, 2006) and 1-(4-chlorophenyl)-3-(2-thienyl)prop-2-en-1-one (Ng *et al.*, 2006) have been reported. In continuation of our work on the crystal structures of chalcones (Yathirajan, Sarojini, Narayana, Ashalatha & Bolte, 2006; Yathirajan, Sarojini, Bindya, Narayana & Bolte, 2006; Yathirajan, Sarojini, Narayana, Bindya & Bolte, 2006), and in view of their importance, we present here the crystal structure of compound (I).



(I)

A perspective view of compound (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November 2005, updated August 2006; *MOGUL*, Version 1.1; Allen, 2002). The aliphatic double bond is *trans* configured. The molecule is essentially planar (r.m.s. deviation for all non-H atoms is 0.056 Å).

Experimental

Compound (I) was synthesized according to the method reported in the literature (Vogel, 1989) in a yield of 85%. The compound was

purified by recrystallization from ethanol. Crystal growth was carried out in an acetone–toluene (50:50 *v*/*v*) solvent mixture by the slow evaporation technique (m.p. 418–420 K). Analysis for $C_{18}H_{14}O_2S$, found (calculated): C 73.40 (73.44), H 4.75 (4.79)%.

Crystal data

$C_{18}H_{14}O_2S$
M_r = 294.35
Monoclinic, $P2_1/c$
a = 3.9155 (3) Å
b = 10.6776 (8) Å
c = 33.521 (3) Å
β = 93.164 (7)°
V = 1399.3 (2) Å^3
Z = 4
D_x = 1.397 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 173 (2) K
Rod, yellow
0.22 × 0.12 × 0.12 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.951, T_{max} = 0.970
10698 measured reflections
2641 independent reflections
2315 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 1.05
2641 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 0.1527P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.036 (5)

H atoms were found in a difference map but they were subsequently refined using a riding model, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C), or C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C_{methyl}). The methyl group was allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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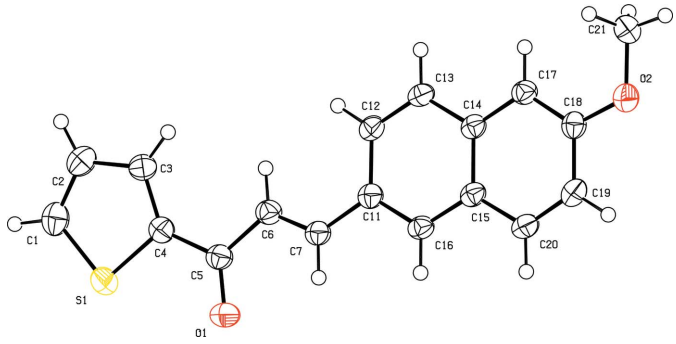

Figure 1
The molecular structure of the title compound, with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

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