Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Abdullah M. Asiri,[a,b] Salman A. Khan[b] and M. Nawaz Tahir[c]*

[a]The Center of Excellence for Advanced Materials Research, King Abdul Aziz University, Jeddah 21589, PO Box 80203, Saudi Arabia, [b]Department of Chemistry, Faculty of Science, King Abdul Aziz University, Jeddah 21589, PO Box 80203, Saudi Arabia, and [c]Department of Physics, University of Sargodha, Sargodha, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

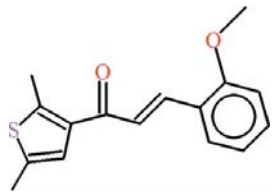
Received 14 August 2010; accepted 14 August 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.102; data-to-parameter ratio = 14.4.

In the title compound, $C_{16}H_{16}O_2S$, the central propenone group is almost planar (r.m.s. deviation = 0.009 Å) and subtends dihedral angles of 8.55 (8) and 16.22 (8)° to the 2-methoxyphenyl and 2,5-dimethylthiophene residues, respectively. The dihedral angle between the ring systems is 23.47 (5)°. In the crystal, molecules are linked by weak C—H···π interactions and aromatic π–π stacking [phenyl ring centroid–centroid separation = 3.6418 (11) Å; thiophene–thiophene ring separation = 3.8727 (9) Å].

Related literature

For background to chalcone derivatives and related crystal structures, see: Asiri *et al.* (2010*a*,*b*,*c*).



Experimental

Crystal data

$C_{16}H_{16}O_2S$
M_r = 272.35
Monoclinic, $C2/c$
a = 26.2978 (6) Å
b = 7.5018 (2) Å
c = 14.7242 (3) Å
β = 105.771 (1)°
V = 2795.45 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 296 K
0.32 × 0.24 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.937, T_{max} = 0.942
10569 measured reflections
2516 independent reflections
2150 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.04
2516 reflections
175 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

*Cg*2 is the centroid of C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···*Cg*2^{i}	0.96	2.89	3.768 (2)	153

Symmetry code: (i) $-x, -y+1, -z+1$.

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* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors would like to thank the Chemistry Department, King Abdul Aziz University, Jeddah, Saudi Arabia, for providing the research facilities and for the financial support of this work *via* grant No. (3–045/430).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5609).

References

Asiri, A. M., Khan, S. A. & Tahir, M. N. (2010*a*). *Acta Cryst.* E**66**, o2099.
Asiri, A. M., Khan, S. A. & Tahir, M. N. (2010*b*). *Acta Cryst.* E**66**, o2133.
Asiri, A. M., Khan, S. A. & Tahir, M. N. (2010*c*). *Acta Cryst.* E**66**, o2259–o2260.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.