Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*E*)-3-(3,4-Dimethoxyphenyl)-1-(2,5-dimethylthiophen-3-yl)prop-2-en-1-one

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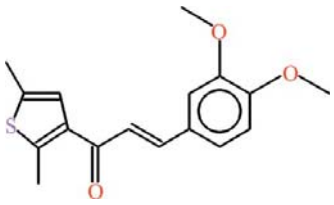
Received 18 July 2010; accepted 22 July 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.106; data-to-parameter ratio = 14.6.

The molecule of the title compound, $C_{17}H_{18}O_3S$, is essentially planar: the phenyl and thiophene rings form a dihedral angle of 2.79 (10)° and they are inclined to the central propenone unit by 6.20 (15) and 4.78 (15)°, respectively. In the crystal, molecules are connected into dimers *via* pairs of C—H···O interactions, generating $R_2^2(14)$ motifs. π–π stacking interactions between the thiophene rings also occur, with a centroid–centroid distance of 3.8062 (12) Å.

Related literature

For background to chalcones, their activity and applications, see: Bandgar *et al.* (2010); Deng *et al.* (2007); Liu *et al.* (2003); Verma *et al.* (2007). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{18}O_3S$
M_r = 302.37
Monoclinic, $P2_1/n$
a = 9.1821 (6) Å
b = 8.3529 (5) Å
c = 20.3443 (13) Å
β = 94.624 (4)°
V = 1555.27 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 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} = 0.868, T_{max} = 0.965
11371 measured reflections
2791 independent reflections
2182 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.106
S = 1.07
2791 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3^{i}	0.93	2.41	3.175 (2)	139

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

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*.

The authors would like to thank the Chemistry Department, King Abdul Aziz University, Jeddah, Saudi Arabia for providing research facilities and for 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: GK2297).

References

Bandgar, B. P., Patil, S. A., Korbad, B. L., Biradar, S. C., Nile, S. N. & Khobragade, C. N. (2010). *Eur. J. Med. Chem.* **45**, 3223–3227.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Deng, J., Sanchez, T., Al-Mawsawi, L. Q., Dayam, R., Yunes, R. A., Garofalo, A., Bolger, M. B. & Neamati, N. (2007). *Bioorg. Med. Chem.* **15**, 4985–5002.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Liu, M., Wilairat, P., Croft, S. L., Tan, A. L. C. & Go, M. (2003). *Bioorg. Med. Chem.* **11**, 2729–2738.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Verma, A. K., Koul, S., Pannu, A. P. S. & Razdan, T. K. (2007). *Tetrahedron*, **63**, 8715–8722.