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(*E*)-1-(2,5-Dimethyl-3-thienyl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one

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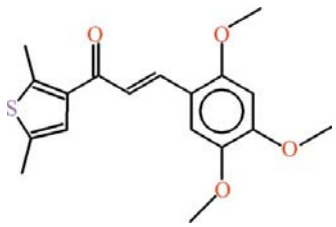
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.113; data-to-parameter ratio = 14.6.

In the title compound, $C_{18}H_{20}O_4S$, the thiophene and benzene rings are oriented at a dihedral angle of 10.83 (11)°. The central chain makes dihedral angles of 1.86 (13) and 9.25 (12)° with the benzene and thiophene rings, respectively. In the crystal, molecules are linked through weak intermolecular C—H···O interactions. π–π interactions are also observed between the benzene rings with a centroid–centroid distance of 3.6832 (12) Å. The slippage between the benzene rings is 0.956 Å.

Related literature

For the biological activity of 1,3-diphenyl-2-propene-1-ones, see: Gökhan-Kelekçi *et al.* (2007); Ducki *et al.* (2009); dos Santos *et al.* (2008); Hussain *et al.* (2009); Dandia *et al.* (2006); Valla *et al.* (2006); Ye *et al.* (2004). For related structures, see: Asiri *et al.* (2009): Hussain *et al.* (2010): Fun *et al.* (2010).



Experimental

Crystal data

$C_{18}H_{20}O_4S$
M_r = 332.40
Tetragonal, $I4_1/a$
a = 19.5263 (5) Å
c = 17.9952 (4) Å
V = 6861.2 (3) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 K
0.26 × 0.18 × 0.16 mm

Data collection

Bruker KAPPA APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.966, T_{max} = 0.975
25995 measured reflections
3106 independent reflections
2225 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.113
S = 1.05
3106 reflections
213 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9*C*···O3^{i}	0.96	2.55	3.209 (3)	126
C14—H14···O4^{ii}	0.93	2.57	3.483 (3)	168

Symmetry codes: (i) $y+\frac{1}{4}, -x-\frac{1}{4}, -z+\frac{3}{4}$; (ii) $-y+\frac{1}{4}, x-\frac{1}{4}, z-\frac{1}{4}$.

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: SI2278).

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