Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*E*)-1-(2,5-Dimethylthiophen-3-yl)-3-(3-nitrophenyl)prop-2-en-1-one

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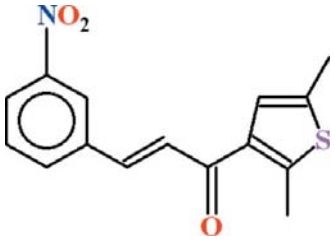
Received 9 November 2011; accepted 11 November 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.117; data-to-parameter ratio = 13.5.

In the title compound, $C_{15}H_{13}NO_3S$, the benzene ring and the five-membered heterocyclic ring are oriented at a dihedral angle of 12.00 (6)°. In the crystal, C—H···O interactions generate two types of cyclic motifs, $R_2^2(14)$ and $R_2^2(26)$, connecting the molecules into tapes extending along [101]. In addition, there are π–π stacking interactions between the benzene and thiophene rings with centroid-centroid distances of 3.7263 (14) and 3.7487 (14) Å.

Related literature

For the synthesis of similar compounds, see: Asiri & Khan (2010, 2011); Kalirajan *et al.* (2009); Patil *et al.* (2009); Sarojini *et al.* (2006). For related structures and background references, see: Asiri *et al.* (2010*a*,*b*). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{15}H_{13}NO_3S$
M_r = 287.32
Monoclinic, $P2_1/c$
a = 7.3802 (5) Å
b = 13.7973 (9) Å
c = 13.4638 (8) Å
β = 96.997 (3)°
V = 1360.77 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 K
0.25 × 0.22 × 0.20 mm

Data collection

Bruker KAPPA APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.945, T_{max} = 0.955
10732 measured reflections
2466 independent reflections
1493 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.117
S = 1.03
2466 reflections
183 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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	2.46	3.373 (3)	168
C15—H15B···O2^{ii}	0.96	2.59	3.339 (4)	135

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+1, -y, -z+1$.

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 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 Abdulaziz University, Jeddah, Saudi Arabia, for providing research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2432).

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