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(2*E*)-3-[4-(Dimethylamino)phenyl]-1-(2,5-dimethyl-3-thienyl)prop-2-en-1-one

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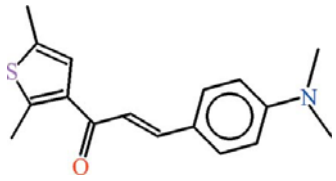
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.049; wR factor = 0.156; data-to-parameter ratio = 14.8.

The asymmetric unit of the title compound, $C_{17}H_{19}NOS$, contains two independent molecules which differ in the dihedral angles between the five- and six-membered rings [12.52 (10) and 4.63 (11)°]. Weak intermolecular C—H···O hydrogen bonds link the two independent molecules into pseudocentrosymmetric dimers. In one molecule, the O atom of the carbonyl group is disordered over two positions in a 0.699 (4):0.301 (4) ratio.

Related literature

For background and related crystal structures, see: Asiri *et al.* (2010*a*,*b*,*c*). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{19}NOS$
M_r = 285.40
Triclinic, $P\overline{1}$
a = 7.7665 (2) Å
b = 12.8624 (4) Å
c = 16.0318 (4) Å
α = 79.917 (1)°
β = 80.029 (2)°
γ = 79.300 (1)°
V = 1532.90 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 K
0.32 × 0.23 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.947, T_{max} = 0.962
22632 measured reflections
5536 independent reflections
3543 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.156
S = 1.02
5536 reflections
373 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O2	0.93	2.48	3.275 (3)	143
C19—H19···O1*A*	0.93	2.52	3.317 (9)	144
C19—H19···O1*B*	0.93	2.48	3.264 (3)	142

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: CV2751).

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