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5-Acetyl-4-methyl-2-(*o*-toluidinyl)-1,3-thiazole

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Key indicators

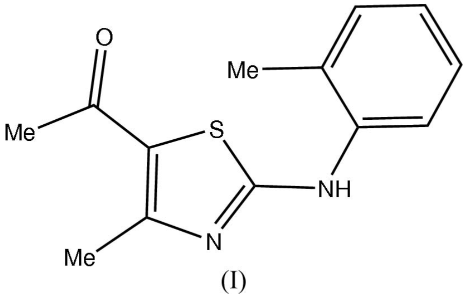
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.122
Data-to-parameter ratio = 16.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{13}H_{14}N_2OS$, the benzene and thiazole rings make a dihedral angle of 73.44 (10)°. The intermolecular N—H···N hydrogen bonds link the molecules into centrosymmetric dimers. The crystal packing is further stabilized by van der Waals forces.

Comment

In the title molecule, (I) (Fig. 1), all bond lengths and angles are in normal ranges (Allen *et al.*, 1987). The geometry of the thiazole ring (Table 1) is close to that observed in its trisubstituted analogue methyl 2-amino-isopropyl-1,3-thiazole-4-carboxylate (Kennedy *et al.*, 2004). The S1/C8/N2/C9/C10/N1/C13 moiety and the C11/C12/O1 acetyl group are essentially coplanar, with a maximum deviation of 0.009 (2) Å for atom N1. The dihedral angle between the thiazole ring and the acetyl fragment is 9.15 (14)°. The benzene and thiazole rings make a dihedral angle of 73.44 (10)°. In the molecule, there is a weak intramolecular C—H···O hydrogen bond (Table 2). Intermolecular N—H···N hydrogen bonds (Table 2) link the molecules into centrosymmetric dimers, arranged parallel to the *ac* face. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.



(I)

Experimental

A solution of *o*-toluidine (1.34 g, 0.01 mol) in acetone (50 ml) was added dropwise to an acetone solution (50 ml) containing an equimolar amount of 3-chloroacetylacetone and ammonium thiocyanate in a two-necked round-bottomed flask. The solution was refluxed for about 1 h. The light-yellow solution was filtered and some colourless crystals were obtained after 5 d of evaporation (yield 80%, m.p. 442.8–442.1 K). ^{1}H NMR: δ 2.34 (3H, *s*, H-7), 2.46 (3H, *s*, H-13), 2.40 (3H, *s*, H-12), 10.10 (H, *s*, NH-2), 7.22–7.50 (CH aromatic, 2–5); ^{13}C NMR: δ 17.8 (C13), 18.3 (C7), 29.9 (C12), 131.6 (C1), 133.6 (C2), 125.3 (C3), 127.6 (C4), 121.5 (C5), 137.8 (C6), 157.5 (C11), 171.5 (C9), 189.3 (C8).

Crystal data

$C_{13}H_{14}N_2OS$
$M_r = 246.32$
Monoclinic, $P2_1/c$
$a = 10.797$ (2) Å
$b = 11.571$ (2) Å
$c = 12.0982$ (16) Å
$\beta = 123.576$ (11)°
$V = 1259.3$ (4) Å^3
$Z = 4$
$D_x = 1.299$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 871 reflections
$\theta = 2.2$–26.5°
$\mu = 0.24$ mm^{-1}
$T = 273$ (2) K
Block, colourless
0.41 × 0.40 × 0.33 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.907$, $T_{\max} = 0.924$
6884 measured reflections
2610 independent reflections
2343 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 26.5°$
$h = -13 \rightarrow 8$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.122$
$S = 1.08$
2610 reflections
157 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0659P)^2 + 0.3401P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.28$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.7269 (16)	N2—C8	1.317 (2)
S1—C9	1.7527 (19)	N2—C10	1.368 (2)
O1—C11	1.219 (3)	C9—C10	1.370 (2)
N1—C8	1.349 (2)		
C8—S1—C9	88.65 (8)	C9—C10—C13	126.24 (17)
C10—C9—C11	128.87 (18)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*B*···O1	0.96	2.50	2.982 (4)	111
N1—H1*A*···N2$^{\rm i}$	0.86	2.17	2.958 (3)	153

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

After their location in a difference Fourier map, all H atoms were positioned geometrically and allowed to ride on the parent C or N atoms, with C—H = 0.93–0.96 Å, N—H = 0.86 Å and $U_{\rm iso}$ = 1.2–1.5$U_{\rm eq}$(parent atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

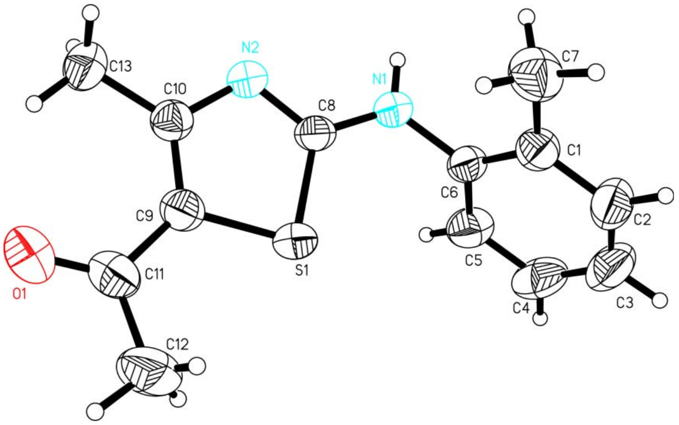


Figure 1
View of (I) with 50% probability displacement ellipsoids.

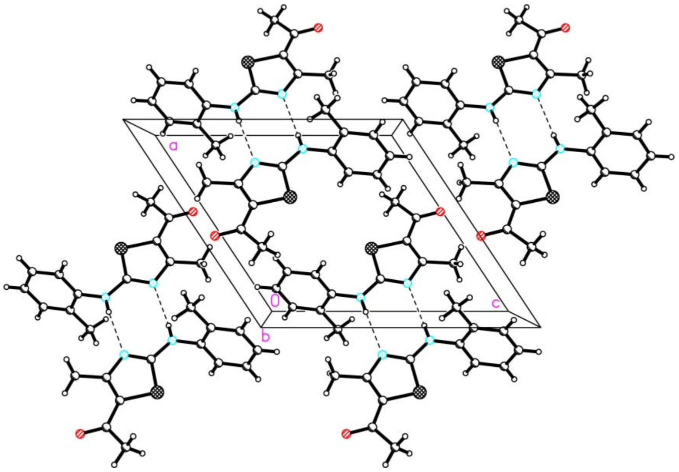


Figure 2
The packing, viewed down the *b* axis. Dashed lines denote intermolecular N—H···N hydrogen bonds.

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