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4-[(1*E*)-Benzylideneamino]-3-methyl-2,4-dihydro-1*H*-1,2,4-triazole-5-thione

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.101
Data-to-parameter ratio = 13.8

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

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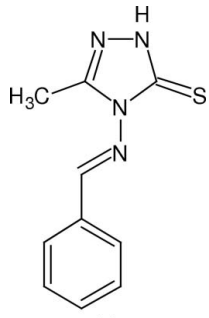
The acyclic C=N double bond of the title compound, $C_{10}H_{10}N_4S$, is *trans* configured. The molecule is almost planar. The angle between the two rings is just 10.25 (7)°. The crystal packing is stabilized by N—H···S hydrogen bonds and π–π interactions.

Comment

Condensed 1,2,4-triazoles are biologically important compounds and are used as starting materials for the synthesis of many heterocycles. Apart from its extensive chemical significance, the 1,2,4-triazole nucleus is found to be associated with diverse medicinal properties and is incorporated in a wide variety of therapeutically interesting drugs (Yathirajan *et al.*, 2005). Recently, some new triazole derivatives have been synthesized as possible anticonvulsants, antidepressants, tranquilizers and plant-growth regulators. Substituted 1,2,4-triazoles have been actively studied as bridging ligands, coordinating through their vicinal N atoms. Complexes containing 1,2,4-triazole ligands possess specific magnetic properties. Other 1,2,4-triazole derivatives have anti-inflammatory activities and some are antifungal agents (Ambalavanan *et al.*, 2003).



(I)

The molecular structure of the title compound, (I), is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.28, November 2006; *Mogul* Version 1.1; Allen, 2002; Bruno *et al.*, 2004). The acyclic C=N double bond is *trans* configured. The angle between the two rings is 10.25 (7)°.

N—H···S hydrogen bonds (Table 1) link the molecules to form centrosymmetric dimers (Fig. 2). The crystal packing is further stabilized by π–π interactions between atom N1 of the the triazole ring and the phenyl ring of a parallel molecule at (1 − *x*, 1 − *y*, 1 − *z*), with an N1···*Cg*(phenyl) [*Cg* is the centroid] distance of 3.649 Å. The molecules crystallize in layers parallel to the (122) plane.

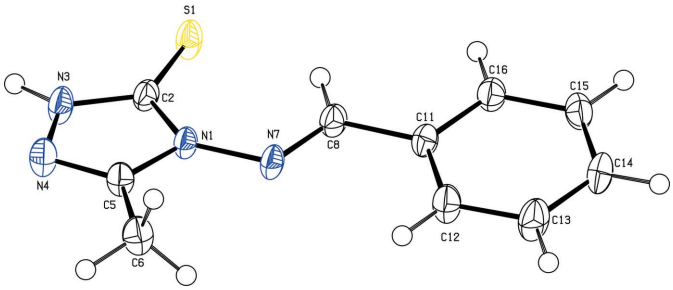


Figure 1
The molecular structure of the title compound, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

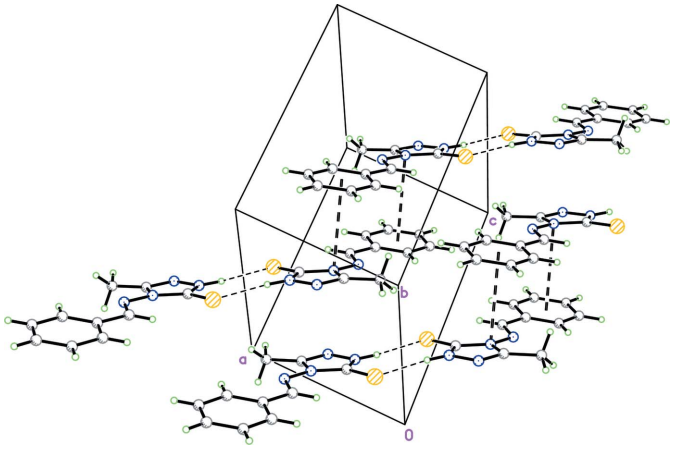


Figure 2
A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines and π–π interactions are shown as bold dashed lines.

Experimental

A mixture of 4-amino-5-methyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione (1.3 g, 0.01 mol) and benzaldehyde (1.06 g, 0.01 mol) in absolute ethanol (25 ml) containing 2 drops of sulfuric acid, was refluxed for about 5 h. On cooling, the solid which separated was filtered off and recrystallized from ethanol (m.p. 468–470 K). Analysis (%) for $C_{10}H_{10}N_4S$, found (calculated): C 54.91 (55.02), H 4.48 (4.62), N 5.52 (25.67), S 14.55 (14.69).

Crystal data

$C_{10}H_{10}N_4S$
M_r = 218.28
Triclinic, $P\overline{1}$
a = 6.9007 (9) Å
b = 7.3551 (10) Å
c = 11.2501 (17) Å
α = 75.288 (11)°
β = 86.091 (12)°
γ = 71.424 (10)°
V = 523.46 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 173 (2) K
0.48 × 0.48 × 0.36 mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.878, T_{max} = 0.906
5717 measured reflections
1957 independent reflections
1820 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 1.06
1957 reflections
142 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···S1^{i}	0.94 (2)	2.38 (2)	3.3093 (14)	172 (2)

Symmetry code: (i) $-x, -y+1, -z+2$.

All H atoms were found in a difference map. The H atom bonded to N was refined freely. The remaining H atoms were refined using a riding model, with C—H distances ranging from 0.95 to 0.99 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C$_{methyl}$). The methyl group was allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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