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N-[4-(*N*,*N*-Diethylamino)benzylidene]-4-phenyl-5-(1*H*-1,2,4-triazol-1-yl)thiazol-2-amine

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.115
Data-to-parameter ratio = 16.0

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

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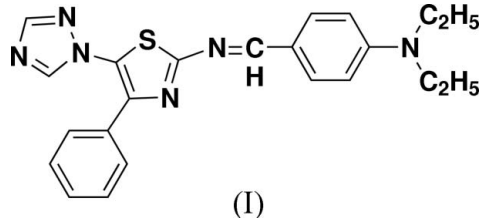
The title compound, $C_{22}H_{22}N_6S$, has been synthesized as a potent fungicidal agent and its crystal structure investigated. The dihedral angles between the plane of the thiazole ring and those of the triazole, phenyl and substituted phenyl rings are 53.0 (2), 37.5 (3) and 14.6 (2)°, respectively.

Comment

Thiazoles exhibit a wide variety of biological activities as antitumour, antifungal, antibiotic and antiviral agents (Hodgetts & Kershaw, 2002). In our previous work, we have synthesized some novel 2-aminothiazole derivatives by incorporating a triazole ring into 2-aminothiazole derivatives in order to improve the biological activity of the parent compounds (Shao *et al.*, 2004). We have recently designed and synthesized the title compound, (I), as part of our continuing investigation into potentially potent fungicides and report its structure here (Fig. 1).



(I)

The title compound contains four planar rings, namely a thiazole (*P*1), a triazole (*P*2), a phenyl (*P*3) and a substituted phenyl (*P*4). The dihedral angles between *P*1 and *P*2, *P*3 and *P*4 are 53.0 (2), 37.5 (3) and 14.6 (2)°, respectively. The C11—N5 distance [1.389 (3) Å] is slightly longer than the corresponding distance in 2-amino-4-(2,5-dichlorophenyl)-5-(1*H*-1,2,4-triazol-1-yl)-1,3-thiazole [1.339 (3) Å; Shao *et al.*, 2004]. The C11—N5—C12—C13 torsion angle is 177.70 (18)°, indicating that the substituted phenyl ring and the thiazole ring have a *trans* configuration.

Experimental

Three drops of piperidine were added to a mixture of 4-phenyl-5-(1*H*-1,2,4-triazol-1-yl)-thiazol-2-yl-amine (0.49 g, 2 mmol) and 4-*N*,*N*-diethylaminobenzaldehyde (0.36 g, 2 mmol) in anhydrous benzene. The solution was then refluxed for 8 h while being monitored using thin-layer chromatography. The solvent was concentrated under reduced pressure at low temperature and the precipitate was filtered and recrystallized from ethanol. Single crystals of (I), suitable for X-ray analysis, were obtained by slow diffusion of petroleum ether and ethyl acetate (3:1).

Crystal data

$C_{22}H_{22}N_6S$
M_r = 402.53
Monoclinic, $P2_1/c$
a = 9.0753 (16) Å
b = 20.924 (4) Å
c = 11.518 (2) Å
β = 108.639 (3)°
V = 2072.5 (6) Å^3
Z = 4
D_x = 1.290 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2309 reflections
θ = 2.4–23.4°
μ = 0.18 mm^{-1}
T = 294 (2) K
Parallelepiped, yellow
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.969, T_{max} = 0.969
11567 measured reflections
4220 independent reflections
2444 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 26.4°
$h = -11 \rightarrow 11$
$k = -26 \rightarrow 21$
$l = -14 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
S = 1.00
4220 reflections
264 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C3	1.719 (2)	N4—C4	1.382 (2)
S1—C11	1.738 (2)	N5—C12	1.287 (3)
N1—C2	1.312 (3)	N5—C11	1.389 (3)
N1—C1	1.355 (3)	N6—C16	1.365 (3)
N2—N3	1.368 (2)	N6—C19	1.466 (3)
N3—C2	1.341 (3)	C3—C4	1.363 (3)
N3—C3	1.415 (2)	C4—C5	1.478 (3)
N4—C11	1.304 (3)	C12—C13	1.437 (3)
C3—S1—C11	88.17 (10)	C4—C3—S1	111.68 (15)
C2—N1—C1	101.58 (19)	C3—C4—N4	113.82 (18)
C1—N2—N3	101.45 (18)	C3—C4—C5	127.39 (18)
C2—N3—N2	109.08 (17)	N4—C11—N5	128.6 (2)
C2—N3—C3	129.98 (18)	N4—C11—S1	115.10 (16)
C11—N4—C4	111.22 (18)	N5—C12—C13	123.3 (2)
C12—N5—C11	117.26 (18)	N5—C12—H12	118.4
N2—N3—C3—C4	−126.5 (2)	C12—N5—C11—S1	−169.54 (16)
N4—C4—C5—C6	−144.2 (2)	C11—N5—C12—C13	177.70 (18)
C4—N4—C11—N5	−175.45 (19)	N5—C12—C13—C18	−174.0 (2)

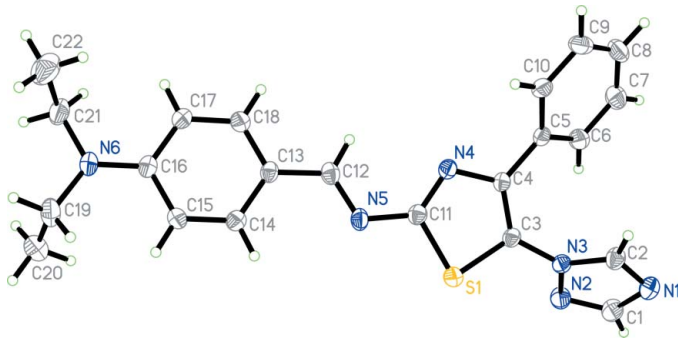


Figure 1
A view of the title compound, with displacement ellipsoids drawn at the 30% probability level.

All H atoms were placed in calculated positions, with C—H = 0.93 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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