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3-Benzyl-4-phenyl-1*H*-1,2,4-triazole-5(4*H*)-thione

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.039
wR factor = 0.109
Data-to-parameter ratio = 9.3

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

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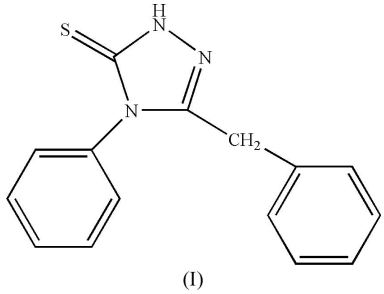
The title compound, $C_{15}H_{13}N_3S$, was prepared by the reaction of 1-(2-chloroethyl)benzene with hydrazine and phenyl isothiocyanate. Packing is stabilized by N—H···S intermolecular hydrogen bonds and C—H···π interactions.

Comment

Compounds containing the 1*H*-1,2,4-triazole group and its derivatives have attracted much interest because they exhibit some fungicidal activity and plant-growth regulating activity (Xu *et al.*, 2002); they also show antibacterial activity against *Puccinia recondite* and root-growth regulation for cucumber (Zhao *et al.*, 1998). In a search for new triazole compounds with higher bioactivity, we have synthesized the title compound, (I), and describe its structure here.



(I)

In (I), bond lengths and angles are normal (Table 1). The dihedral angles formed by the triazole plane with the C1–C6

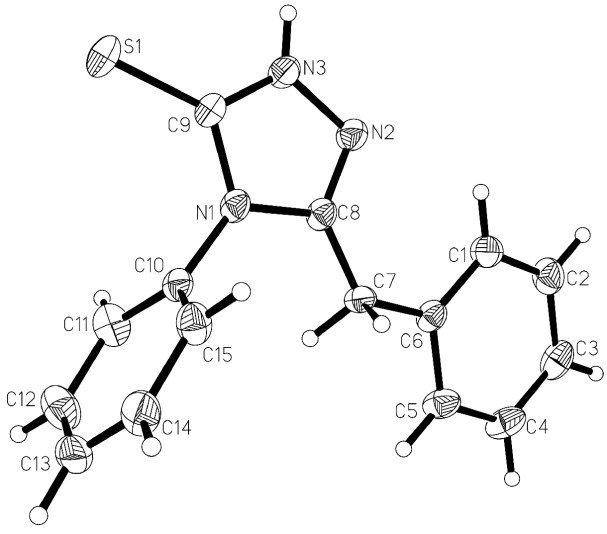


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

and C10–C15 phenyl rings are 15.3 (1) and 85.2 (1)°, respectively. The dihedral angle between the two phenyl rings is 80.8 (1)°. The crystal structure is stabilized by N—H···S intermolecular hydrogen bonds and C—H···π interactions (Table 2).

Experimental

The title compound was prepared by the reaction of 1-(2-chloroethyl)benzene (2.81 g, 0.02 mol) with hydrazine (0.60 g, 0.02 mol) and phenyl isothiocyanate (2.24 g, 0.02 mol) in NaOH solution (30 ml). Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from propanol solution at room temperature.

Crystal data

$C_{15}H_{13}N_3S$
M_r = 267.34
Monoclinic, *Cc*
a = 15.277 (3) Å
b = 11.810 (2) Å
c = 8.6360 (17) Å
β = 121.79 (3)°
V = 1324.4 (6) Å^3
Z = 4
D_x = 1.341 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 4–14°
μ = 0.23 mm^{-1}
T = 295 (2) K
Block, yellow
0.35 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
1763 measured reflections
1605 independent reflections
1506 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.0°
$h = -1 \rightarrow 18$
$k = -1 \rightarrow 14$
$l = -10 \rightarrow 9$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
S = 1.08
1605 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0827P)^2 + 0.2246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.073 (6)
Absolute structure: Flack (1983), 1450 Friedel pairs
Flack parameter = 0.03 (2)

Table 1
Selected bond lengths (Å).

S1—C9	1.687 (3)	N2—C8	1.295 (4)
N1—C9	1.380 (4)	N2—N3	1.383 (4)
N1—C8	1.386 (3)	N3—C9	1.325 (4)
N1—C10	1.436 (4)		

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C10–C15 phenyl rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···S1^{i}	0.86	2.58	3.279 (3)	139
C14—H14A···Cg1^{ii}	0.93	2.74	3.565 (2)	149
C3—H3B···Cg2^{iii}	0.93	2.79	3.690 (2)	164

Symmetry codes: (i) $x, -y, \frac{1}{2}+z$; (ii) $x, y, z-1$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{3}{2}+z$.

H atoms were positioned geometrically and allowed to ride on their attached atoms, with C—H = 0.93–0.97 Å and $U_{iso} = 1.2U_{eq}$(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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