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4-Phenyl-1-(1-phenylethylidene)thiosemicarbazide

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Key indicators

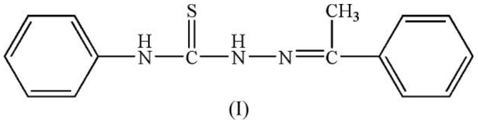
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.054
wR factor = 0.169
Data-to-parameter ratio = 16.7

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

The title compound, $C_{15}H_{15}N_3S$, was prepared by the reaction of acetophenone and hydrazine with phenylisothiocyanate. In the molecule, all bond lengths and angles are within normal ranges. The two phenyl rings make a dihedral angle of 61.6 (2)°. The crystal packing is stabilized by van der Waals forces.

Comment

Thiosemicarbazides are able to form complexes with biological activities (Shen *et al.*, 1998). Thiourea derivatives have been successfully screened for various biological activities (Antholine & Taketa, 1982), and some of them have shown promising anti-HIV properties (Mao *et al.*, 1999). As ligands with potential S and N donors, thiosemicarbazides are important due to their multifunctional coordination modes, *viz*. monodentate (*N*- or *S*-) or bidentate (*N*- and *S*-). In our search for new ligands of this type, we have synthesized the title compound, (I), and describe its structure here.



(I)

In (I) (Fig. 1), the bond lengths and angles (Table 1) are usual for this type of compound (Ji *et al.*, 2002). The mean planes *p*1 (S1/N2/N3/C9/C10) and *p*2 (N1/N2/C6/C7/C8) make a dihedral angle of 7.1 (2)°. The dihedral angles formed by phenyl ring C1–C6 with *p*1 and *p*2 are 20.5 (2) and 18.2 (3)°, respectively, while the dihedral angles C10–C15/*p*1 and C10–C15/*p*2 are 53.7 (1) and 60.6 (2)°, respectively. The dihedral angle between the two phenyl rings is 61.6 (2)°. The crystal packing (Fig. 2) is stabilized by van der Waals forces.

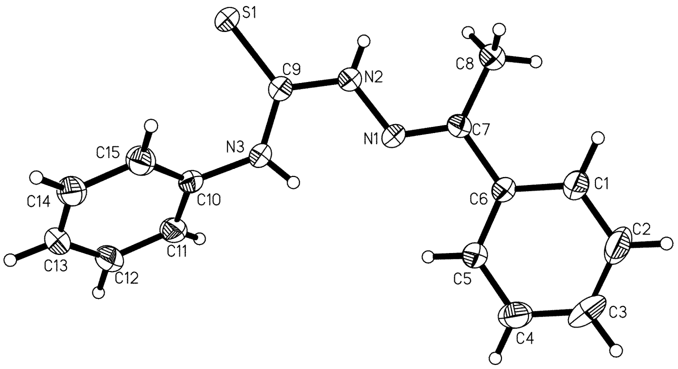


Figure 1
View of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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Experimental

The title compound was prepared by the reaction of hydrazine (0.02 mol) and acetophenone (0.02 mol) with phenyl isothiocyanate (0.02 mol). Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from acetone solution at room temperature.

Crystal data

$C_{15}H_{15}N_3S$
$M_r = 269.36$
Triclinic, $P\overline{1}$
$a = 5.9250\ (12)$ Å
$b = 10.514\ (2)$ Å
$c = 11.567\ (2)$ Å
$\alpha = 103.54\ (3)^\circ$
$\beta = 91.10\ (3)^\circ$
$\gamma = 90.19\ (3)^\circ$
$V = 700.4\ (2)$ Å^3
$Z = 2$
$D_x = 1.277$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 4$–26°
$\mu = 0.22$ mm^{-1}
$T = 295\ (2)$ K
Block, colourless
$0.25 \times 0.20 \times 0.18$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
3302 measured reflections
3014 independent reflections
1352 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\rm max} = 27.0^\circ$
$h = 0 \rightarrow 7$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 13$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.169$
$S = 1.02$
3014 reflections
180 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0732P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.33$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C9	1.680 (3)	N2—C9	1.356 (4)
N1—C7	1.279 (4)	N3—C9	1.343 (4)
N1—N2	1.385 (4)	N3—C10	1.425 (4)
C7—N1—N2	118.9 (3)	C9—N3—C10	127.5 (3)
C9—N2—N1	119.4 (3)		
N2—N1—C7—C6	176.9 (3)	C9—N3—C10—C15	−54.9 (5)
C1—C6—C7—N1	−160.9 (3)	C9—N3—C10—C11	128.9 (4)
C5—C6—C7—N1	17.9 (5)		

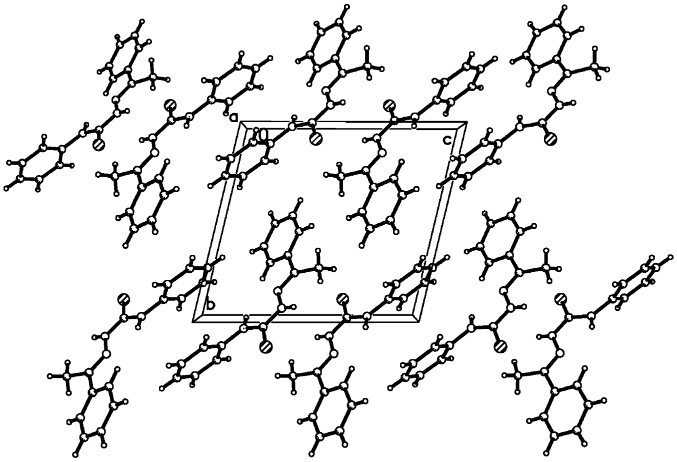

Figure 2
The crystal packing of (I), viewed down the *a* axis.

After their location in a difference Fourier map, the C-bound H atoms were placed in calculated positions and allowed to ride on their parent atoms, with C—H = 0.93–0.96 Å and $U_{\rm iso} = 1.2$–$1.5U_{\rm eq}$(C). The N-bound H atoms were also located in a difference Fourier map and were refined isotropically.

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, 1990); 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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