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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.056
 wR factor = 0.180
Data-to-parameter ratio = 17.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

1-(Furan-2-ylmethylene)-4-phenylthiosemicarbazide

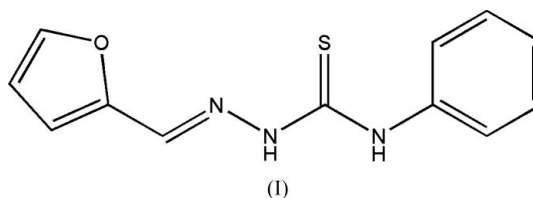
In the molecule of the title compound, $\text{C}_{12}\text{H}_{11}\text{N}_3\text{OS}$, the dihedral angle between the planar rings is $59.4(2)^\circ$. The structure is stabilized by intramolecular $\text{N}-\text{H}\cdots\text{N}$ and intermolecular $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds. Intermolecular $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds link the independent molecules into dimers.

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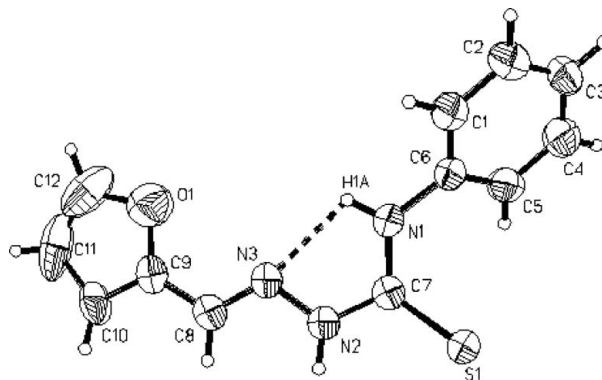
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Comment

Thiosemicarbazide is interesting because of the formation of complexes with biological activities (Shen *et al.*, 1998). Some substituted thiourea derivatives have shown interesting biological effects, including anti-HIV properties (Mao *et al.*, 1999), and thiourea derivatives have also been successfully screened for various biological actions (Antholine & Taketa, 1982). As a ligand with potential S- and N-atom donors, thiosemicarbazide is interesting because of the structural chemistry of its multifunctional coordination modes (*N*-monodentate, *S*-monodentate or *N:S*-bidentate). In order to investigate further this kind of ligand, we synthesized the title compound, (I), and describe its structure here.



In the molecule of (I) (Fig. 1), the bond lengths and angles are in normal ranges (Allen *et al.*, 1987; Ji *et al.*, 2002). The dihedral angle between the planar rings is $59.4(2)^\circ$.

**Figure 1**

The molecular structure of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

The crystal structure of (I) is stabilized by intramolecular N—H···N and intermolecular N—H···S hydrogen bonds (Table 1). Intermolecular N—H···S hydrogen bonds link the independent molecules into dimers (Fig. 2). Dipole–dipole and van der Waals interactions are also effective in the molecular packing in the crystal structure.

Experimental

The title compound was prepared by the reaction of hydrazine (1.0 g, 20 mmol) and furfural (1.9 g, 20 mmol) with phenyl isothiocyanate (2.7 g, 20 mmol). Single crystals suitable for X-ray measurements were obtained by recrystallization from an acetone solution at room temperature (yield 3.9 g, 79.4%; m.p. 402–404 K).

Crystal data

$C_{12}H_{11}N_3OS$	$V = 611.6 (2) \text{ \AA}^3$
$M_r = 245.31$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.332 \text{ Mg m}^{-3}$
$a = 5.8810 (12) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.878 (2) \text{ \AA}$	$\mu = 0.25 \text{ mm}^{-1}$
$c = 11.186 (2) \text{ \AA}$	$T = 296 (2) \text{ K}$
$\alpha = 71.45 (3)^\circ$	Block, brown
$\beta = 83.18 (3)^\circ$	$0.35 \times 0.25 \times 0.25 \text{ mm}$
$\gamma = 88.95 (3)^\circ$	

Data collection

Enraf–Nonius CAD-4 diffractometer	1882 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.010$
Absorption correction: none	$\theta_{\text{max}} = 27.0^\circ$
2889 measured reflections	3 standard reflections every 100 reflections
2675 independent reflections	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1127P)^2 + 0.1125P]$
$R[F^2 > 2\sigma(F^2)] = 0.056$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.180$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
2675 reflections	$\Delta\rho_{\text{min}} = -0.52 \text{ e \AA}^{-3}$
154 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots N3$	0.86	2.19	2.607 (3)	109
$N2-H2A\cdots S1^i$	0.86	2.54	3.382 (2)	166

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

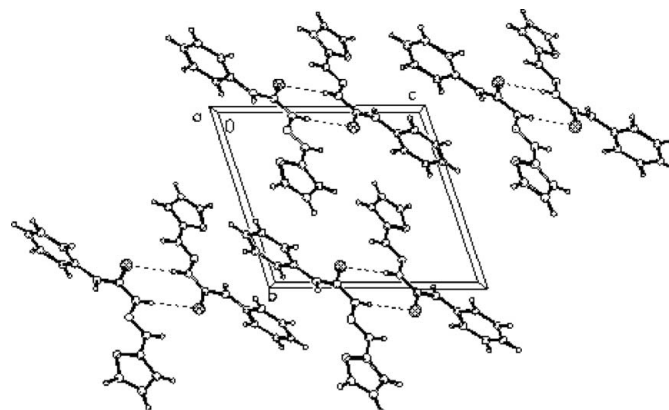


Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

H atoms were positioned geometrically, with N—H = 0.86 \AA and C—H = 0.93 \AA , and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

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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