Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Phenyl-1-(propan-2-ylidene)thiosemicarbazide

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.119
Data-to-parameter ratio = 18.4

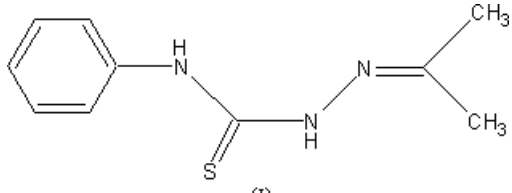
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 10 January 2005
Accepted 7 February 2005
Online 12 February 2005

The title compound, $C_{10}H_{13}N_3S$, was prepared by the reaction of acetone with hydrazine and phenyl isothiocyanate. The molecular structure and crystal packing are stabilized by N—H···N and N—H···S hydrogen bonds.

Comment

There is considerable current interest in the coordination chemistry of transition metals with the Schiff base family of ligands (Kovacic, 1967). In most cases, it was found that chelation of the bases with salts of transition metals occurred readily, whereas those Schiff bases which are prepared from *ortho*-hydroxy-substituted aldehydes readily form chelates similar to the type obtained from 8-hydroxyquinoline and its derivatives. In our study of these ligands, we synthesized the title compound, (I), and present its structure (Fig. 1).



(I)

The relatively short S1—C7 bond length (Table 1) indicates its double-bond character. Atoms S1/C7/N1/N2/N3 and C10/C9/C8/N2/N3 define the mean planes *p*1 and *p*2, respectively; the dihedral angle between them is 13.6 (1)°. The dihedral angles formed by the plane of the phenyl ring with *p*1 and *p*2 are 38.3 (2) and 39.6 (2)°, respectively. The molecular structure of (I) and the crystal packing are stabilized by intramolecular N—H···N and intermolecular N—H···S hydrogen

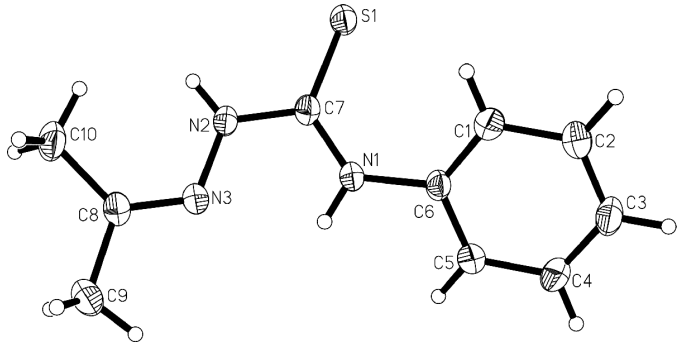


Figure 1
View of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

bonds (Table 2). The relatively short distance of 3.733 (2) Å between atom C9 and the centroid (*Cg*) of the phenyl ring at $(1 + x, y, z)$ may indicate the presence of a C—H$\cdots\pi$ interaction (H9*C*$\cdots$*Cg* = 2.79 Å and C9—H9*C*$\cdots$*Cg* = 166°).

Experimental

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

Crystal data

$C_{10}H_{13}N_3S$
M_r = 207.29
Monoclinic, $P2_1/c$
a = 9.0660 (18) Å
b = 10.283 (2) Å
c = 11.889 (2) Å
β = 99.07 (3)°
V = 1094.5 (4) Å^3
Z = 4
D_x = 1.258 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 4–14°
μ = 0.26 mm^{-1}
T = 295 (2) K
Block, yellow
0.35 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
3104 measured reflections
2352 independent reflections
1937 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.0°
$h = -1 \rightarrow 10$
$k = -1 \rightarrow 12$
$l = -14 \rightarrow 14$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.119
S = 1.04
2352 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 0.3495P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.035 (4)

Table 1
Selected bond lengths (Å).

S1—C7	1.6816 (18)	N2—C7	1.359 (2)
N1—C7	1.337 (2)	N2—N3	1.385 (2)
N1—C6	1.420 (2)	N3—C8	1.279 (2)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1*B*$\cdots$N3	0.86	2.13	2.571 (2)	111
N2—H2*A*$\cdots$S1^{i}	0.86	2.68	3.4713 (16)	154

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

H atoms were positioned geometrically and allowed to ride on their attached atoms, with N—H and C—H distances of 0.86 and 0.93–0.96 Å, respectively, and with U_{iso}(H) = 1.2 or 1.5U_{eq} of the parent atom.

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).

The authors thank the Natural Science Foundation of Shandong Province (No. Y2002B06).

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