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1-[1-(3-Nitrophenyl)ethylidene]thiosemicarbazide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.079
wR factor = 0.257
Data-to-parameter ratio = 16.2

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

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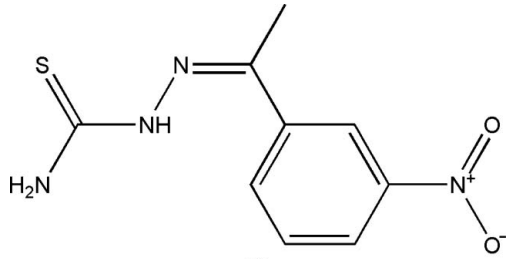
The title compound, $C_9H_{10}N_4O_2S$, was prepared by the reaction of thiosemicarbazide with 1-(3-nitrophenyl)ethanone at room temperature. The crystal packing is stabilized by van der Waals forces.

Comment

Schiff bases have been used extensively as ligands in the field of coordination chemistry (Jian *et al.*, 2005, 2006). Schiff bases show potential as antimicrobial and anticancer agents (Tarafder *et al.*, 2000; Deschamps *et al.*, 2003) and so have biochemical and pharmacological applications. The recent growing interest in Schiff bases is also due to their ability to form intramolecular hydrogen bonds by electron coupling between acid-base centers (Rozwadowski *et al.*, 1999). We report here the crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1 and Table 1), the C7—N2 bond length is a little shorter than that of a standard C═N bond (Liu *et al.*, 2002). The C9—S1 bond length is within the range of values observed for a C═S bond (Jian *et al.*, 2005, 2006). Atoms C7/N2/N3/N4/C9/S1 and 01/02/N1/C1/C2/C3/C4/C5/C6 define the mean planes *p*1 and *p*2, respectively, with a dihedral angle between them of 16.70 (1)°. Atoms S1/N2/N3/N4/C9 define the mean plane *p*3. The dihedral angle between *p*3 and benzene ring C1–C6 is 60.03 (1)°, and those made by *p*1 and *p*3, and by *p*3 and *p*2 are 46.66 (1) and 60.78 (1)°, respectively.

Experimental

A mixture of thiosemicarbazide (0.02 mol) and hydrochloric acid (0.02 mol) was stirred in ethanol (30 ml) for 10 min. *o*-Fluoroacetophenone (0.02 mol) was then added and the mixture was stirred at 293 K for 2 h to afford the title compound (2.28 g, yield 54%). Single crystals suitable for X-ray measurements were obtained by recrystallization from acetone at room temperature.

Crystal data

$C_9H_{10}N_4O_2S$
M_r = 238.27
Orthorhombic, *Pbca*
a = 13.756 (3) Å
b = 8.0690 (16) Å
c = 19.835 (4) Å
V = 2201.6 (8) Å^3
Z = 8
D_x = 1.438 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 (2) K
Block, yellow
0.25 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
4617 measured reflections
2345 independent reflections
1172 reflections with $I > 2\sigma(I)$
R_{int} = 0.118
θ_{max} = 27.0°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.257
S = 0.98
2345 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1483P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Table 1
Selected bond lengths (Å).

S1—C9	1.698 (5)	N2—C7	1.282 (6)
O1—N1	1.216 (6)	N2—N3	1.387 (5)
O2—N1	1.233 (6)	N3—C9	1.345 (6)
N1—C1	1.458 (7)	N4—C9	1.321 (6)

H atoms were positioned geometrically and allowed to ride on their parent 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 1.5 times U_{eq} of the parent atoms.

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).

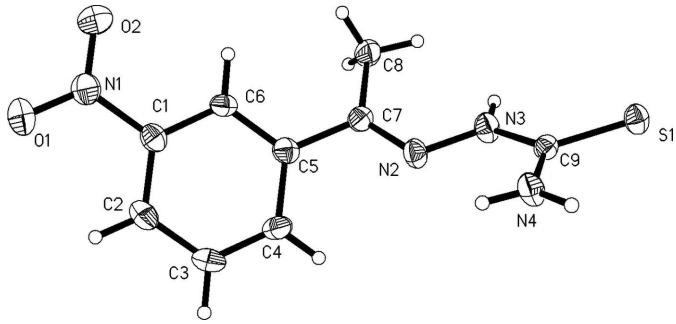


Figure 1
The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

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