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1-[1-(2-Fluorophenyl)ethylidene]thiosemicarbazide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.138
Data-to-parameter ratio = 15.8

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

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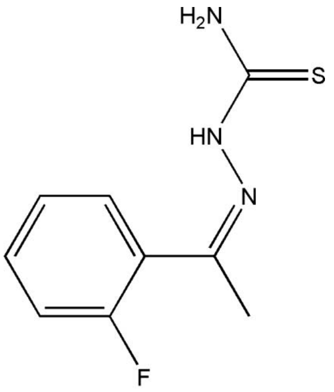
The title compound, $C_9H_{10}FN_3S$, was prepared by the reaction of thiosemicarbazide with *o*-fluoacetophenone at room temperature. The packing is stabilized by intra- and intermolecular hydrogen bonds.

Comment

Schiff bases have been used extensively as ligands in the field of coordination chemistry (Jian *et al.*, 2006). They are potential 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 centres (Rozwadowski *et al.*, 1999). Here we report the crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), the C7—N1 bond length [1.284 (2) Å] is a little shorter than that expected for a typical C═N bond (Liu *et al.*, 2002). The C—S bond length [1.691 (2) Å] is comparable with the values observed for a C═S double bond (Jian *et al.*, 2005). The dihedral angles formed by the mean plane through the N1/N2/C7/C8 system with the thiosemicarbazide fragment (S1/N2/N3/C9) and the benzene ring are 11.62 (10) and 49.99 (9)°, respectively.

The molecular structure is stabilized by intramolecular C—H···F and N—H···N hydrogen bonds (Table 1). In the crystal packing, the molecules are linked into two-dimensional layers by intermolecular N—H···S hydrogen-bond interactions (Table 1).

Experimental

A mixture of thiosemicarbazide (0.02 mol) and hydrochloric acid (0.02 mol) was stirred in ethanol (30 ml) for 10 min, then *o*-fluoroacetophenone (0.02 mol) was added and the resulting 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 slow evaporation of an acetone solution at room temperature.

Crystal data

$C_9H_{10}FN_3S$
$M_r = 211.26$
Monoclinic, $P2_1/c$
$a = 6.4920$ (13) Å
$b = 18.589$ (4) Å
$c = 8.6000$ (17) Å
$\beta = 97.03$ (3)°
$V = 1030.0$ (4) Å^3
$Z = 4$
$D_x = 1.362$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.29$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.25 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
2381 measured reflections
2193 independent reflections
1591 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\rm max} = 27.0°$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.138$
$S = 1.09$
2193 reflections
139 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0808P)^2 + 0.1009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.40$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.28$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···N1	0.85 (3)	2.22 (2)	2.595 (2)	107 (2)
C8—H8A···F1	0.96	2.53	2.979 (3)	109
N2—H2A···S1$^{\rm i}$	0.85 (3)	2.82 (3)	3.665 (2)	173 (2)
N3—H3A···S1$^{\rm ii}$	0.92 (2)	2.59 (2)	3.506 (2)	169 (2)

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x, -y+1, -z+1$.

H atoms attached to N atoms were located in a difference Fourier map and refined freely. All other H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.96 Å and with $U_{\rm iso}$(H) = 1.2 or 1.5 times $U_{\rm eq}$(C).

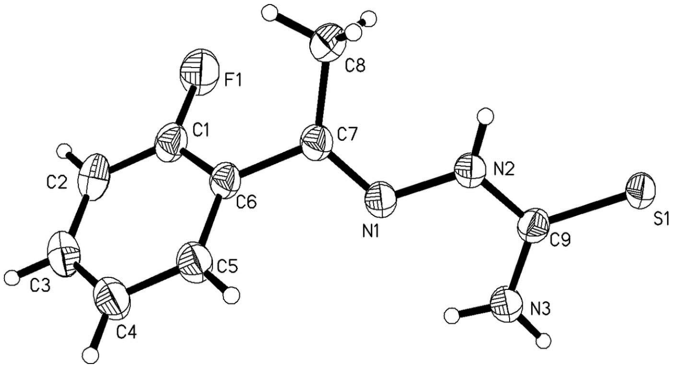


Figure 1
The molecular structure and atom-labelling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

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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