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2-[(5-Methylthiazol-2-ylimino)methyl]phenol

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In the title molecule, $C_{11}H_{10}N_2OS$, the benzene ring makes a dihedral angle of 6.4 (2)° with the thiazole ring. The expected electron delocalization is observed in the –C—N═CH– imino system.

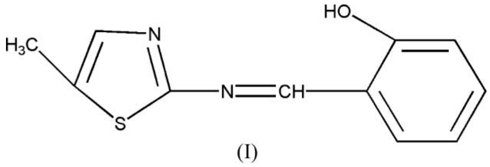
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.064
wR factor = 0.156
Data-to-parameter ratio = 13.4

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

Comment

Schiff bases can exhibit antibacterial, anticancer, anti-inflammatory and antitoxic activities, and sulfur-containing Schiff bases are particularly effective (Canan *et al.*, 2000). Consequently, many sulfur-containing Schiff bases have been synthesized and their crystal structures determined, including 2-[(4-hydroxyphenyl)iminomethyl]thiophene (Kazak *et al.*, 2000) and *N*-benzylidene-4-(ferrocenyl)-5-(1*H*-1,2,4-triazol-1-yl)-1,3-thiazol-2-amine (Yu *et al.*, 2005). In an extension of this area of research, we report here the synthesis and structure determination of a related compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1 and key torsion angles are listed in Table 1. The dihedral angle between the rings is 6.4 (2)°. The N2—C4 bond [1.391 (4) Å] is shorter than a typical C—N bond length [ca 1.443 (4) Å], but longer than a typical double C═N bond [ca 1.269 (2) Å], while the N2—C5 bond [1.2788(4 Å] is slightly longer than a typical double C═N bond, indicating the presence of electron delocalization in the vicinity of atoms C4, N2 and C5. The other bond lengths and angles in (I) have standard distances (Allen *et al.*, 1987). There is an intramolecular O—H···N hydrogen bond (Table 2), which may stabilize the molecular conformation.

Experimental

Under a nitrogen atmosphere, a mixture of 2-amino-5-methylthiazole (10 mmol), anhydrous Na_2SO_4 (3.0 g) and salicyaldehyde (10 mmol) in anhydrous ethanol (30 ml) was refluxed for about 6 h, yielding a yellow precipitate. The product was collected by vacuum filtration and washed with ethanol. The crude soild was recrystallized from CH_2Cl_2 (100 ml) and washed with water (2 × 10 ml) and brine (10 ml). After drying over Na_2SO_4, the solvent was removed under vacuum, and a yellow solid was isolated in 90% yield (1.73 g). Yellow single crystals of the compound suitable for X-ray analysis were grown from a hexane–anhydrous ethanol (4:1) solution by slow evaporation at room temperature over a period of about a week.

Crystal data

$C_{11}H_{10}N_2OS$
$M_r = 218.28$
Monoclinic, $P2_1/c$
$a = 13.991$ (2) Å
$b = 5.0713$ (8) Å
$c = 17.0873$ (17) Å
$\beta = 119.956$ (8)°
$V = 1050.4$ (3) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.28$ mm^{-1}
$T = 298$ (2) K
0.39 × 0.31 × 0.25 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.899$, $T_{\max} = 0.933$
5127 measured reflections
1850 independent reflections
1730 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.156$
$S = 1.18$
1850 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.39$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

Table 1
Selected torsion angles (°).

C4—S1—C2—C3	−0.5 (3)	C5—N2—C4—S1	−179.1 (2)
C4—S1—C2—C1	178.2 (3)	C2—S1—C4—N1	0.6 (3)
C4—N1—C3—C2	0.0 (5)	C2—S1—C4—N2	−177.9 (2)
C3—N1—C4—N2	177.9 (3)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.82	1.90	2.624 (3)	147

H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2—H = 0.93 Å, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(parent atom), Csp^3—H = 0.96 Å, with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(parent atom), and O—H = 0.82 Å, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(parent atom).

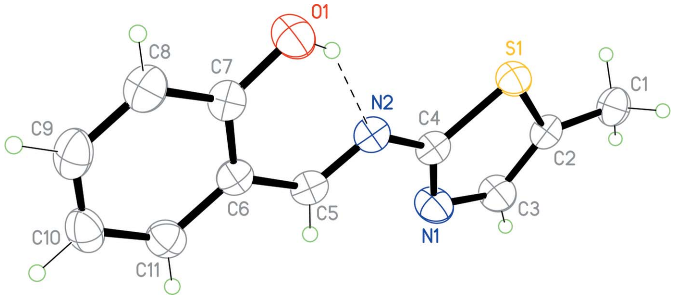


Figure 1
The molecular structure of (I), with the atom numbering, showing displacement ellipsoids drawn at the 30% probability level. The dashed line indicates the hydrogen bond.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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