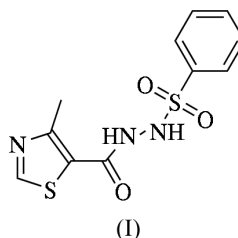


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Key indicators

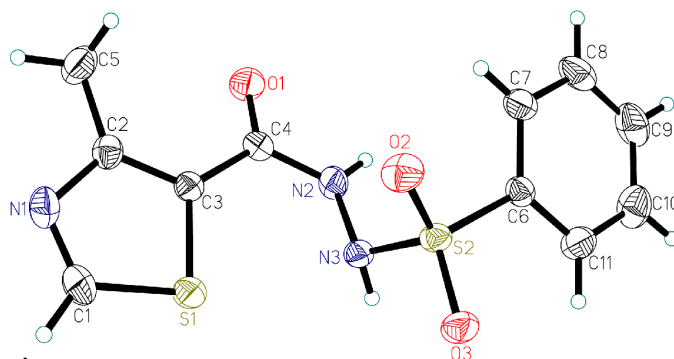
Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.034
wR factor = 0.094
Data-to-parameter ratio = 12.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*N'*-(Benzenesulfonyl)-4-methylthiazole-5-carbohydrazideCrystals of the title compound, $\text{C}_{11}\text{H}_{11}\text{N}_3\text{O}_3\text{S}_2$, were obtained from the sulfonylation reaction of 4-methylthiazole-5-carbohydrazide with benzenesulfonyl chloride. The crystal packing is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds.

Comment

The title compound, (I) (Fig. 1), is a derivative of benzenesulfohydrazide (Chekhlov & Martynov, 1988) and is a ligand with the *O,N,S*-donors of an *N'*-arylsulfonylthiazole-5-carbohydrazide derivative. It coordinates to transition metals and rare-earth metals. Some of the arylsulfohydrazine derivatives show potential bioactivities (Darias *et al.*, 1995; Dutta *et al.*, 1986; Ariesan *et al.*, 1971).In (I), all bond lengths and angles are normal (Table 1). The crystal packing is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds (Table 2 and Fig. 2).

Experimental

The title compound (2.4 g, 80% yield) was obtained from the sulfonylation reaction of 4-methylthiazole-5-carbohydrazide (1.3 g) with benzenesulfonyl chloride (2.0 g) in the presence of pyridine (25 ml). Colorless single crystals of (I) suitable for diffraction analysis were obtained from an ethyl acetate solution after one week.

**Figure 1**
The structure of the title compound, showing 40% probability displacement ellipsoids and the atom-numbering scheme.

Crystal data

$C_{11}H_{11}N_3O_3S_2$
 $M_r = 297.35$
 Monoclinic, $P2_1/c$
 $a = 10.5593$ (9) Å
 $b = 12.8979$ (11) Å
 $c = 10.1875$ (9) Å
 $\beta = 111.703$ (2)°
 $V = 1289.11$ (19) Å³
 $Z = 4$

$D_x = 1.532$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 3203 reflections
 $\theta = 5.2$ – 55.9 °
 $\mu = 0.42$ mm⁻¹
 $T = 293$ (2) K
 Prism, colorless
 $0.45 \times 0.42 \times 0.39$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.430$, $T_{\max} = 0.850$
 6372 measured reflections

2275 independent reflections
 1995 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$
 $\theta_{\text{max}} = 25.0$ °
 $h = -12 \rightarrow 12$
 $k = -15 \rightarrow 15$
 $l = -10 \rightarrow 12$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.094$
 $S = 1.04$
 2275 reflections
 181 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.1299P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.28$ e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.018 (2)

Table 1

Selected torsion angles (°).

C2–N1–C1–S1	1.3 (3)	C1–S1–C3–C4	–172.02 (17)
C3–S1–C1–N1	–1.07 (19)	S2–C6–C7–C8	–174.53 (15)
C1–N1–C2–C3	–0.9 (3)	C6–C7–C8–C9	–1.4 (3)
C1–N1–C2–C5	179.52 (19)	C7–C8–C9–C10	–0.5 (3)
N1–C2–C3–C4	172.68 (17)	C8–C9–C10–C11	2.2 (4)
N1–C2–C3–S1	0.1 (2)	C9–C10–C11–C6	–2.0 (3)
C5–C2–C3–S1	179.66 (17)	C7–C6–C11–C10	0.2 (3)
C1–S1–C3–C2	0.51 (15)		

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3–H3 ⁱ ⋯N1 ⁱ	0.89 (2)	2.00 (2)	2.866 (2)	164 (2)
N2–H2 ⁱⁱ ⋯O3 ⁱⁱ	0.88 (2)	2.18 (2)	2.963 (2)	148 (2)

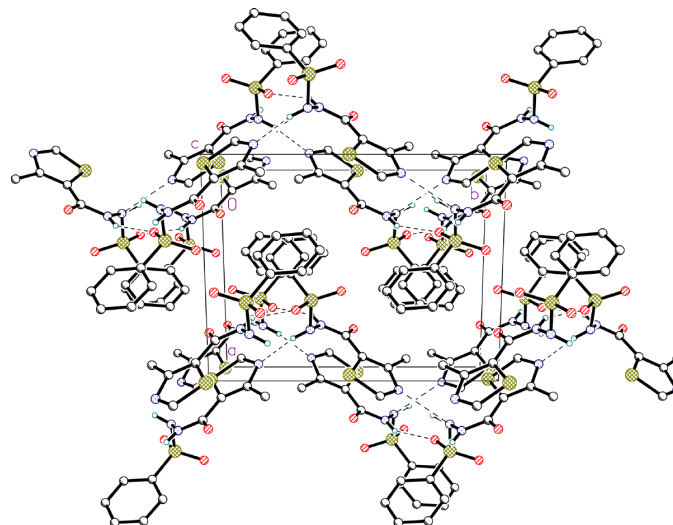
Symmetry codes: (i) $2-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$.

Figure 2

A packing diagram of the title compound, viewed down the c axis. Intermolecular N–H⋯O and N–H⋯N hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted.

The positions of atoms H2 and H3 were found in a Fourier difference map and refined freely; other H atoms were placed in calculated positions and allowed to ride on their parent atoms at distances in the range 0.93–0.96 Å for CH groups. Isotropic displacement parameters were set at 1.2 to 1.5 times U_{eq} of the parent atom.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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