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2′-(2-Thienylmethylidene)-2-hydroxybenzohydrazide

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Key indicators

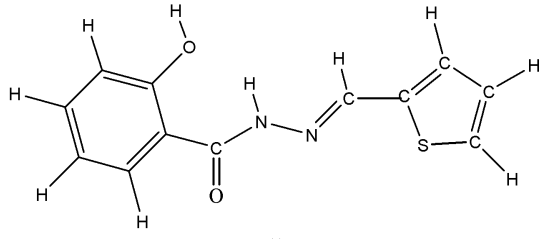
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.157
Data-to-parameter ratio = 14.7

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

The title compound, $C_{12}H_{10}N_2O_2S$, was synthesized by the reaction of 2-hydroxybenzoylhydrazine with 2-thiophenecarboxaldehyde in ethanol. The crystal structure involves intermolecular O—H···O and intramolecular N—H···O hydrogen bonds.

Comment

Some benzoylhydrazone compounds possess bacteriostatic activity. This type of compound has wide application in the treatment of tuberculosis and also exhibits fungicidal activity (Edwards *et al.*, 1975). Furthermore, the hydrazonecarbonyl is a structural motif showing bioactivity (Zhi *et al.*, 2003). In order to search for more effective antibacterial medicines, we have synthesized the title compound, (I).



(I)

The molecule is essentially planar, with an r.m.s. deviation of 0.0048 Å. An intermolecular O—H···O hydrogen bond is observed linking the hydroxyl H atom with the carbonyl group of an adjacent molecule. In addition, an intramolecular O—H···N hydrogen bond linking the amide NH group with the hydroxyl group, forming a six-membered ring (Fig. 2), is also found.

Experimental

2-Hydroxybenzoylhydrazine (0.02 mol, 3.04 g) was dissolved in anhydrous ethanol (50 ml) at room temperature. 2-Thiophenecarbox-

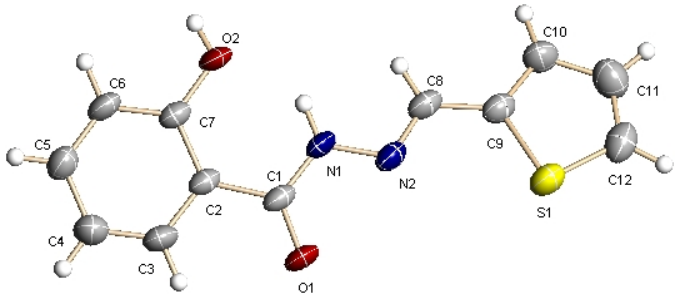


Figure 1
The structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 30% probability level.

aldehyde (0.02 mol, 1.88 g) was added and the mixture refluxed for 2 h. The precipitate was collected by filtration and washed with ethanol. The product was recrystallized from ethanol and dried under reduced pressure, giving the title compound. The compound (2.5 mmol, 0.62 g) was dissolved in dimethylformamide (30 ml) and kept at room temperature for 30 d, after which colorless block-shaped single crystals formed and were collected and washed with distilled water.

Crystal data

$C_{12}H_{10}N_2O_2S$
M_r = 246.28
Monoclinic, $P2_1/n$
a = 4.9785 (6) Å
b = 21.127 (2) Å
c = 10.9004 (13) Å
β = 102.209 (2)°
V = 1120.6 (2) Å^3
Z = 4
D_x = 1.460 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2410 reflections
θ = 5.4–54.4°
μ = 0.28 mm^{-1}
T = 293 (2) K
Block, colorless
0.51 × 0.26 × 0.17 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.871, T_{max} = 0.955
6565 measured reflections
2442 independent reflections
1945 reflections with $I > 2\sigma(I)$
R_{int} = 0.073
θ_{max} = 27.0°
$h = -6 \rightarrow 6$
$k = -18 \rightarrow 26$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.157
S = 1.04
2442 reflections
166 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0957P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected bond lengths (Å).

S1—C12	1.682 (2)	N1—C1	1.344 (3)
S1—C9	1.702 (2)	N1—N2	1.368 (2)
O1—C1	1.228 (2)	N2—C8	1.268 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.781 (17)	1.918 (18)	2.6681 (19)	161 (3)
N1—H1···O2	0.80 (2)	2.01 (2)	2.625 (2)	134.5 (19)

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

All H atoms (except H1, H2 and H8) were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 Å (C—H), with U_{iso}(H) = 1.2U_{eq}(parent atom). Atoms H1, H2 and H8 were located in a difference Fourier map and their parameters were refined. The N1—H1 distance is 0.80 (2) Å, the O2—H2 distance is 0.781 (17) Å and the C8—H8 distance is 0.89 (3) Å.

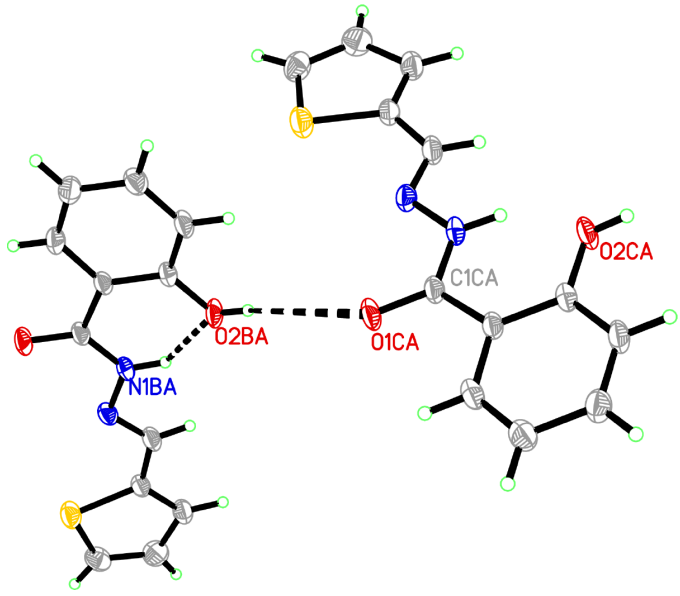


Figure 2
Intermolecular and intramolecular hydrogen bonds (dashed lines).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT* and *SHELXTL* (Bruker, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Bruker (2002). *SMART* (Version 5.62), *SAINT* (Version 6.02), *SADABS* (Version 2.03) and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Edwards, E. I., Epton, R. & Marr, G. (1975). *J. Organomet. Chem.* **85**, C23—C25.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Zhi, J. F., Bin, Z., Su, H. W. & Zheng, M. L. (2003). *Chin. J. Appl. Chem.* **20**, 365–367.