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5-[(2-Hydroxyphenyl)methyleneamino]-1,3,4-thiadiazole-2(3*H*)-thione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.085
Data-to-parameter ratio = 13.3

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

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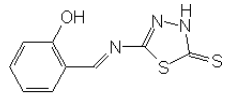
The title compound, $C_9H_7N_3OS_2$, is essentially planar and features an intramolecular O—H···N interaction. Centrosymmetrically related molecules associate *via* N—H···S contacts.

Comment

The biological versatility of compounds incorporating a thiadiazole ring is well known (Kumar & Nizamuddin, 1988; Yadav *et al.*, 1989). In this connection, it was thought of interest to combine a Schiff base with a thiadiazole ring system. Thus, the synthesis and structure of a new compound, namely 5-[(2-hydroxyphenyl)methyleneamino]-1,3,4-thiadiazole-2(3*H*)-thione, (I), is reported.



(I)

The molecular structure of (I) (Fig. 1 and Table 1) has two approximately parallel fragments linked by a Schiff base, with the dihedral angle between the aromatic and thiadiazole rings being 1.0 (1)°. The C9—S2 bond length of 1.662 (3) Å is approximately 0.08 Å shorter than the C9—S1 bond length, confirming the presence of the thione. There is an O1—H···N1 intramolecular hydrogen-bonding interaction, such that the O···N separation is 2.614 (3) Å, with an O—H···N angle of 146°. Centrosymmetrically related molecules associate *via* N3—H···S2^{i} contacts [H···S2^{i} = 2.44° and N3···S2^{i} = 3.291 (2) Å; symmetry code: (i) $-1-x$, $1-y$, $1-z$]. There is also a C7—H···O1^{ii} interaction with a C7···O1^{ii} separation of 3.391 (3) Å [symmetry code: (ii) x, $\frac{1}{2}-y$, $\frac{1}{2}+z$].

Further work investigating the biological activity of (I) is in progress.

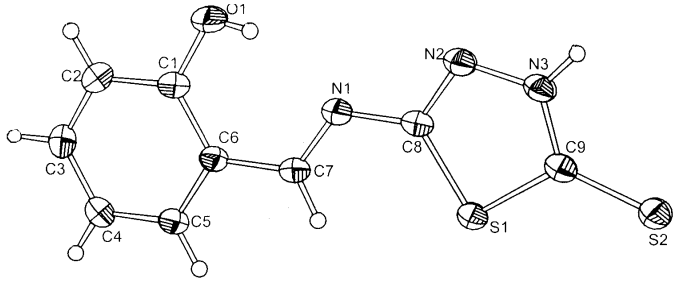


Figure 1
View of (I), showing displacement ellipsoids at the 30% probability level.

Experimental

(I) was prepared using a procedure similar to a reported method (Wang *et al.*, 1999). Yellow single crystals were obtained by recrystallization from a hot ethanol solution of the compound. IR (KBr): 3390 (*s*), 3260 (*s*), 1615 (*s*) cm^{-1}. ^1H NMR (DMSO-d_6): δ 14.58 (1H, *m*), 8.89 (1H, *m*), 11.15 (1H, *s*), 7.02–7.98 (4H, *s*). Calculated for $C_9H_7N_3OS_2$: C 45.23, H2.68, N 17.50%; found: C 45.53, H 2.97, N 17.74%.

Crystal data

$C_9H_7N_3OS_2$
M_r = 237.30
Monoclinic, $P2_1/c$
a = 6.587 (3) Å
b = 13.723 (5) Å
c = 11.758 (5) Å
β = 99.183 (6)°
V = 1049.2 (7) Å^3
Z = 4
D_x = 1.502 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 662 reflections
θ = 3.1–26.0°
μ = 0.48 mm^{-1}
T = 293 (2) K
Block, yellow
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995; Sheldrick, 1996)
T_{min} = 0.841, T_{max} = 0.890
2862 measured reflections
1822 independent reflections
1440 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.1°
$h = -4 \rightarrow 7$
$k = -14 \rightarrow 16$
$l = -12 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.085
S = 1.06
1822 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 0.2779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C9	1.743 (2)	N1—C7	1.288 (3)
S1—C8	1.762 (2)	N1—C8	1.372 (3)
S2—C9	1.662 (3)	N3—C9	1.339 (3)
N2—C8	1.296 (3)	C1—O1	1.354 (3)
N2—N3	1.358 (3)		
C7—N1—C8	121.16 (19)	N1—C7—C6	121.8 (2)

The H atoms were included in the riding-model approximation.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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