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(E)-2-Methoxy-6-(thiazol-2-ylimino-methyl)phenol

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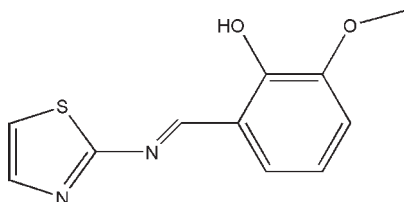
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.044; wR factor = 0.110; data-to-parameter ratio = 13.2.

The title compound, $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_2\text{S}$, displays an *E* configuration about the $\text{C}=\text{N}$ bond. The mean planes of the thiazole and benzene rings make a dihedral angle of 9.32 (18)°. Intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds are found in the crystal structure.

Related literature

For general background to Schiff bases, see: Lv *et al.* (2006); Tarafder *et al.* (2002); Zhou *et al.* (2009).



Experimental

Crystal data

 $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_2\text{S}$ $M_r = 234.27$ Monoclinic, $C2/c$ $a = 24.765$ (3) Å $b = 4.9619$ (8) Å $c = 20.238$ (2) Å $\beta = 117.931$ (2)° $V = 2197.2$ (5) Å³ $Z = 8$ Mo $K\alpha$ radiation $\mu = 0.28$ mm⁻¹ $T = 298$ K $0.29 \times 0.18 \times 0.17$ mm

Data collection

Siemens SMART CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\min} = 0.923$, $T_{\max} = 0.954$

5338 measured reflections

1920 independent reflections

1139 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.034$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.044$ $wR(F^2) = 0.110$ $S = 1.02$

1920 reflections

146 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.19$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{N2}$	0.82	1.91	2.627 (3)	146

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2011).

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supplementary materials

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(*E*)-2-Methoxy-6-(thiazol-2-yliminomethyl)phenol

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Comment

Schiff bases have been extensively researched because of their important applications in coordination chemistry, catalysis and biological processes. (Lv *et al.* 2006, Tarafder *et al.* 2002, Zhou *et al.* 2009). Owing to the importance of these Schiff base analogue compounds, we report here the crystal structure of the title compound, C₁₁H₁₀N₂O₂S₁, (I).

The title compound was prepared by the condensation reaction of 2-hydroxy-3-methoxybenzaldehyde with an equimolar quantity of thiazol-2-amine (Fig. 1). The structure of (I) shows a *trans* or *E* configuration about the C=N bond. The dihedral angle between the mean planes of the thiazole and benzene rings is 9.32 (18)°. Intramolecular O1—H1···N2 hydrogen bonds are found in the crystal structure. Crystal packing is stabilized mainly by van der Waals interactions (Fig. 2).

Experimental

2-hydroxy-3-methoxybenzaldehyde (10 mmol) was added to a ethanolic solution of thiazol-2-amine (10 mmol). Then, the reaction mixture was heated for 2 h under reflux. After filtration a yellow powder was obtained. Suitable crystals for X-ray diffraction were obtained by recrystallization from methanol. Anal. Calcd (%) for C₁₁H₁₀N₂O₂S₁ (Mr = 234.27): C, 56.40; H, 4.30; N, 11.96; O, 13.66; S, 13.69. Found (%): C, 56.38; H, 4.35; N, 11.90; O, 13.69; S, 13.68.

Refinement

All the nonhydroxy H atoms were placed in geometrically idealized positions (C_{methyl}—H = 0.96 and all other C—H = 0.93 Å) and constrained to ride on their parent atoms, with with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{C8})$. The H atoms attached to oxygen atoms were located from the Fourier difference map and refined isotropically.

Figures

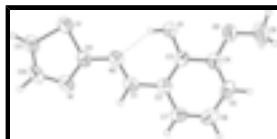


Fig. 1. The molecular structure of the title molecule, with 50% probability displacement ellipsoids. An O—H···N intramolecular hydrogen bond is shown as a dashed line.



Fig. 2. The molecular packing of the title compound, viewed along the *b* axis. Intramolecular hydrogen bonds are shown as dashed lines.

(E)-2-Methoxy-6-(thiazol-2-yliminomethyl)phenol

Crystal data

$C_{11}H_{10}N_2O_2S$	$F_{000} = 976$
$M_r = 234.27$	$D_x = 1.416 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: $-C 2yc$	Cell parameters from 1208 reflections
$a = 24.765 (3) \text{ \AA}$	$\theta = 3.3\text{--}21.9^\circ$
$b = 4.9619 (8) \text{ \AA}$	$\mu = 0.28 \text{ mm}^{-1}$
$c = 20.238 (2) \text{ \AA}$	$T = 298 \text{ K}$
$\beta = 117.931 (2)^\circ$	Block, colorless
$V = 2197.2 (5) \text{ \AA}^3$	$0.29 \times 0.18 \times 0.17 \text{ mm}$
$Z = 8$	

Data collection

Siemens SMART CCD area-detector diffractometer	1920 independent reflections
Radiation source: fine-focus sealed tube	1139 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.034$
$T = 298 \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.9^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -29 \rightarrow 26$
$T_{\text{min}} = 0.923$, $T_{\text{max}} = 0.954$	$k = -5 \rightarrow 5$
5338 measured reflections	$l = -24 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 1.8745P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
1920 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
146 parameters	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.10966 (12)	1.1575 (6)	0.46446 (14)	0.0681 (8)

N2	0.09882 (10)	0.9199 (5)	0.35514 (12)	0.0495 (6)
O1	0.09126 (9)	0.6986 (4)	0.23318 (10)	0.0582 (6)
H1	0.0833	0.8091	0.2575	0.087*
O2	0.13089 (10)	0.3468 (4)	0.17130 (12)	0.0687 (6)
S1	0.01303 (4)	1.2680 (2)	0.34433 (5)	0.0702 (3)
C1	0.14555 (13)	0.7692 (6)	0.39241 (16)	0.0512 (7)
H1A	0.1658	0.7842	0.4442	0.061*
C2	0.16805 (12)	0.5776 (6)	0.35747 (15)	0.0458 (7)
C3	0.13974 (12)	0.5484 (6)	0.27981 (16)	0.0457 (7)
C4	0.16169 (13)	0.3571 (6)	0.24731 (17)	0.0514 (8)
C5	0.21123 (14)	0.2002 (6)	0.29263 (19)	0.0608 (9)
H5	0.2259	0.0724	0.2714	0.073*
C6	0.23948 (14)	0.2313 (7)	0.3698 (2)	0.0642 (9)
H6	0.2730	0.1246	0.3999	0.077*
C7	0.21848 (13)	0.4170 (6)	0.40180 (18)	0.0576 (8)
H7	0.2378	0.4370	0.4535	0.069*
C8	0.14472 (19)	0.1291 (7)	0.1360 (2)	0.0966 (13)
H8A	0.1856	0.1494	0.1428	0.145*
H8B	0.1164	0.1291	0.0835	0.145*
H8C	0.1415	-0.0380	0.1578	0.145*
C9	0.08023 (13)	1.1000 (6)	0.39362 (16)	0.0500 (7)
C10	0.07640 (17)	1.3433 (7)	0.48042 (19)	0.0747 (10)
H10	0.0900	1.4100	0.5286	0.090*
C11	0.02367 (16)	1.4240 (7)	0.42374 (18)	0.0678 (9)
H11	-0.0031	1.5471	0.4274	0.081*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0747 (18)	0.082 (2)	0.0432 (15)	0.0066 (16)	0.0239 (14)	-0.0087 (14)
N2	0.0487 (15)	0.0539 (15)	0.0471 (14)	-0.0046 (13)	0.0234 (12)	-0.0034 (13)
O1	0.0626 (13)	0.0576 (13)	0.0500 (12)	0.0124 (11)	0.0227 (10)	-0.0032 (10)
O2	0.0912 (17)	0.0617 (15)	0.0625 (14)	0.0129 (12)	0.0438 (13)	-0.0047 (12)
S1	0.0629 (5)	0.0897 (7)	0.0526 (5)	0.0103 (5)	0.0227 (4)	-0.0114 (5)
C1	0.0543 (18)	0.0540 (19)	0.0412 (16)	-0.0111 (16)	0.0188 (15)	-0.0017 (15)
C2	0.0451 (17)	0.0415 (17)	0.0498 (18)	-0.0068 (14)	0.0214 (14)	0.0009 (14)
C3	0.0438 (17)	0.0396 (17)	0.0557 (19)	-0.0002 (14)	0.0250 (15)	0.0022 (15)
C4	0.0572 (19)	0.0481 (19)	0.058 (2)	-0.0037 (16)	0.0343 (17)	0.0010 (16)
C5	0.061 (2)	0.049 (2)	0.088 (3)	0.0018 (16)	0.048 (2)	0.0035 (18)
C6	0.0493 (19)	0.059 (2)	0.079 (3)	0.0027 (17)	0.0254 (18)	0.0138 (19)
C7	0.0516 (19)	0.056 (2)	0.0569 (19)	-0.0035 (16)	0.0189 (16)	0.0046 (17)
C8	0.162 (4)	0.068 (3)	0.084 (3)	0.021 (3)	0.077 (3)	-0.002 (2)
C9	0.0572 (18)	0.0507 (18)	0.0481 (18)	-0.0063 (15)	0.0298 (15)	-0.0029 (15)
C10	0.093 (3)	0.083 (3)	0.051 (2)	0.000 (2)	0.036 (2)	-0.018 (2)
C11	0.075 (2)	0.078 (2)	0.060 (2)	0.004 (2)	0.0391 (19)	-0.0082 (19)

Geometric parameters (\AA , $^\circ$)

N1—C9	1.300 (3)	C3—C4	1.401 (4)
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supplementary materials

N1—C10	1.372 (4)	C4—C5	1.378 (4)
N2—C1	1.284 (3)	C5—C6	1.389 (4)
N2—C9	1.398 (3)	C5—H5	0.9300
O1—C3	1.351 (3)	C6—C7	1.361 (4)
O1—H1	0.8200	C6—H6	0.9300
O2—C4	1.361 (3)	C7—H7	0.9300
O2—C8	1.423 (4)	C8—H8A	0.9600
S1—C11	1.689 (3)	C8—H8B	0.9600
S1—C9	1.704 (3)	C8—H8C	0.9600
C1—C2	1.443 (4)	C10—C11	1.333 (4)
C1—H1A	0.9300	C10—H10	0.9300
C2—C3	1.397 (4)	C11—H11	0.9300
C2—C7	1.397 (4)		
C9—N1—C10	108.6 (3)	C7—C6—H6	119.8
C1—N2—C9	119.1 (2)	C5—C6—H6	119.8
C3—O1—H1	109.5	C6—C7—C2	120.5 (3)
C4—O2—C8	117.2 (3)	C6—C7—H7	119.8
C11—S1—C9	89.58 (16)	C2—C7—H7	119.8
N2—C1—C2	123.0 (3)	O2—C8—H8A	109.5
N2—C1—H1A	118.5	O2—C8—H8B	109.5
C2—C1—H1A	118.5	H8A—C8—H8B	109.5
C3—C2—C7	119.3 (3)	O2—C8—H8C	109.5
C3—C2—C1	121.0 (3)	H8A—C8—H8C	109.5
C7—C2—C1	119.7 (3)	H8B—C8—H8C	109.5
O1—C3—C2	122.8 (3)	N1—C9—N2	126.4 (3)
O1—C3—C4	117.3 (3)	N1—C9—S1	115.3 (2)
C2—C3—C4	119.9 (3)	N2—C9—S1	118.2 (2)
O2—C4—C5	125.7 (3)	C11—C10—N1	116.9 (3)
O2—C4—C3	114.9 (3)	C11—C10—H10	121.5
C5—C4—C3	119.4 (3)	N1—C10—H10	121.5
C4—C5—C6	120.5 (3)	C10—C11—S1	109.5 (3)
C4—C5—H5	119.7	C10—C11—H11	125.2
C6—C5—H5	119.7	S1—C11—H11	125.2
C7—C6—C5	120.4 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots N2	0.82	1.91	2.627 (3)	146

Fig. 1

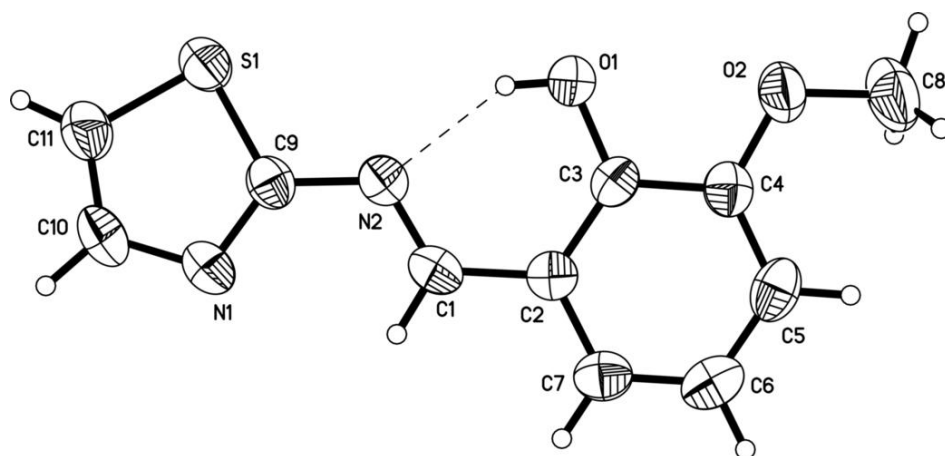


Fig. 2

