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

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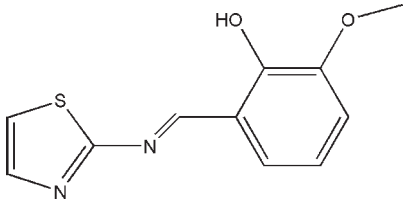
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.110; data-to-parameter ratio = 13.2.

The title compound, $C_{11}H_{10}N_2O_2S$, displays an *E* configuration about the C=N bond. The mean planes of the thiazole and benzene rings make a dihedral angle of 9.32 (18)°. Intramolecular O—H···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

$C_{11}H_{10}N_2O_2S$
M_r = 234.27
Monoclinic, $C2/c$
a = 24.765 (3) Å
b = 4.9619 (8) Å
c = 20.238 (2) Å
β = 117.931 (2)°
V = 2197.2 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 298 K
0.29 × 0.18 × 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_{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
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···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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supporting information

Acta Cryst. (2009). E**65**, o2675 [https://doi.org/10.1107/S1600536809040410]

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

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S1. 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, $C_{11}H_{10}N_2O_2S_1$, (I).

The title compoud 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).

S2. 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 $C_{11}H_{10}N_2O_2S_1$ (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.

S3. 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_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C8). The H atoms attached to oxygen atoms were located from the Fourier differece map and refined isotropically.

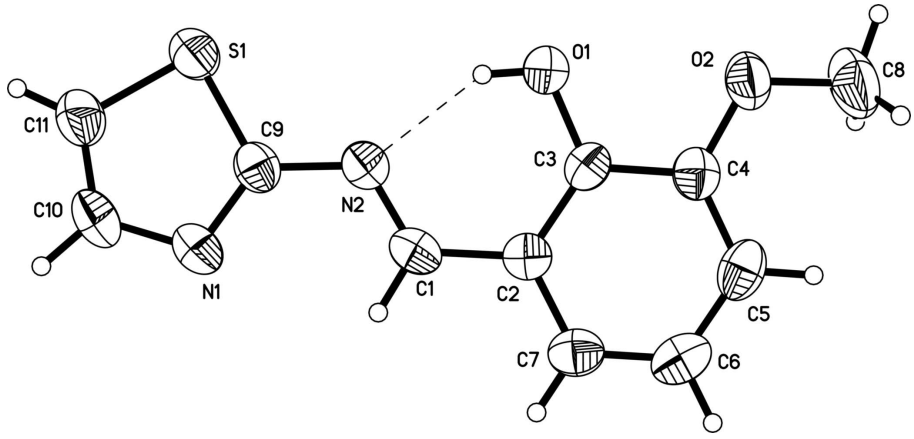

Figure 1

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.

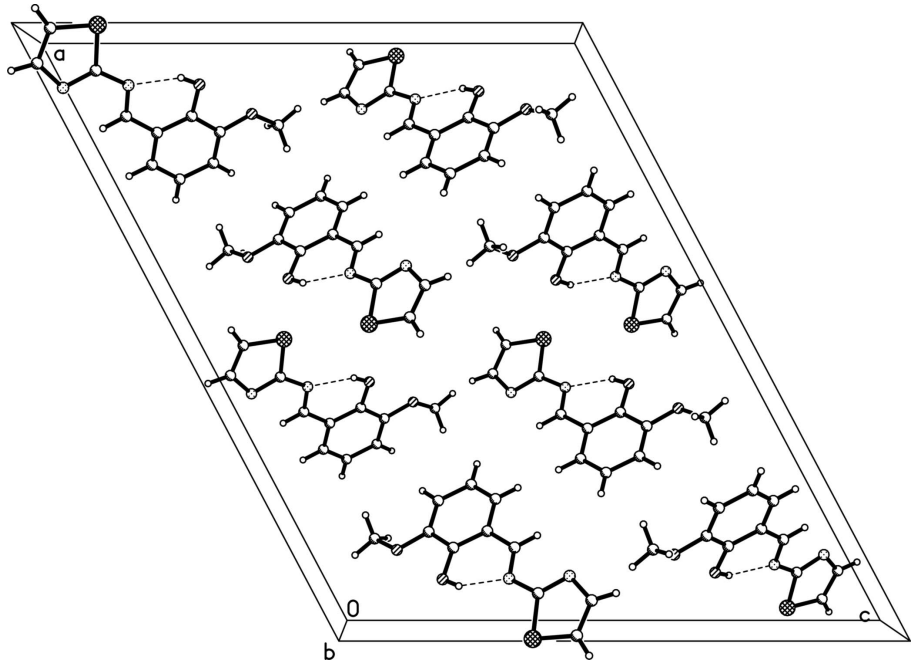

Figure 2

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

$C_{11}H_{10}N_2O_2S$
$M_r = 234.27$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 24.765\ (3)$ Å
$b = 4.9619\ (8)$ Å
$c = 20.238\ (2)$ Å
$\beta = 117.931\ (2)°$
$V = 2197.2\ (5)$ Å^3
$Z = 8$
$F(000) = 976$
$D_x = 1.416$ Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1208 reflections
θ = 3.3–21.9°
μ = 0.28 mm^{-1}
T = 298 K
Block, colorless
0.29 × 0.18 × 0.17 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
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_{int} = 0.034
θ_{max} = 25.0°, θ_{min} = 1.9°
h = −29→26
k = −5→5
l = −24→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.110
S = 1.02
1920 reflections
146 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 1.8745P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{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 (Å²)

	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 (Å, º)

N1—C9	1.300 (3)	C3—C4	1.401 (4)
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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.82	1.91	2.627 (3)	146