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## Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
R factor = 0.050  
wR factor = 0.133  
Data-to-parameter ratio = 14.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 2-(Benzothiazol-2-yliminomethyl)-6-methoxyphenol

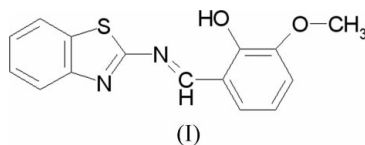
The crystal structure of the title compound,  $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_2\text{S}$ , consists of a dimeric arrangement of molecules linked through  $\text{C5}-\text{H5}\cdots\text{O2}$  and  $\text{O1}-\text{H1}\cdots\text{S1}$  hydrogen bonds.

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## Comment

Aminothiazoles have many applications in both human and veterinary medicine (Lynch *et al.*, 1999). Certain 2-aminobenzothiazole derivatives act on the central nervous system, possess antimicrobial and antibacterial properties, serve as neuroleptic agents, or act as plant growth regulators. In this context, the synthesis of new 2-aminobenzothiazole derivatives is of interest (El'tsov & Mokrushin, 2002). Among the antitumor agents discovered in recent years, the identification of various 2-(4-aminophenyl)benzothiazoles as potent and selective antitumor drugs against breast, ovarian, colon and renal cell lines has stimulated remarkable interest (Usman *et al.*, 2003, Shi *et al.*, 1996).

The molecular structure of the title compound, (I), is shown Fig. 1. The molecule has an approximately planar structure, except for atoms O2, C5 and C2, which deviate from the mean plane of the molecule by 0.187 (3),  $-0.177$  (2) and 0.1634 (18)  $\text{\AA}$ , respectively. The molecule crystallizes in the *E* configuration, with the C7-benzothiazole group and the C9-methoxyphenol group on opposite sides of the  $\text{C8}=\text{N2}$  double bond. This configuration agrees with that commonly found in benzothiazole derivatives (Cannon *et al.*, 2001).

While the  $\text{N2}-\text{C8}$  bond distance [1.283 (3)  $\text{\AA}$ ] is longer than a typical  $\text{N}=\text{C}$  bond distance, the  $\text{N2}-\text{C7}$  single bond length is shorter than reported values (Cannon *et al.*, 2001), which suggests the existence of a delocalized double bond in the benzothiazole moiety. The molecule adopts an extended planar conformation, with torsion angles  $\text{N1}-\text{C7}-\text{N2}-\text{C8} = -9.0$  (4) $^\circ$  and  $\text{C7}-\text{N2}-\text{C8}-\text{C9} = 179.2$  (2) $^\circ$ . Analysis of the bond lengths and angles confirms  $sp^2$  hybridization of all the C and N atoms of the benzothiazole fragment, with all values intermediate between C-C and C-N single and double bonds. There is an  $\text{O1}-\text{H1}\cdots\text{N2}$  intramolecular hydrogen bond within the molecule, while neighboring molecules are linked to each other to form a dimeric structure *via*  $\text{C5}-\text{H5}\cdots\text{O2}^i$  and  $\text{O1}-\text{H1}\cdots\text{S1}^i$  hydrogen bonding [symmetry code: (i)  $1-x, 1-y, 1-z$ ] (Table 2 and Fig. 2). As can be seen from the packing diagram (Fig. 2), the dimers are

approximately parallel to the [101] axis. Dipole–dipole and van der Waals interactions are also effective in the molecular packing in the crystal structure.

## Experimental

A solution of 2-aminobenzothiazole (4 mmol) in *n*-butanol (20 ml) was added dropwise to a hot solution of *o*-vanillin (2-hydroxy-3-methoxybenzaldehyde) (4 mmol) in *n*-butanol (30 ml). The mixture was refluxed for 2 h. The solution was then reduced by evaporation to half-volume (25 ml) and allowed to cool. The precipitated product was filtered off and recrystallized from absolute ethanol. UV/vis ( $C_2H_5OH$ ):  $\lambda_{max}$  ( $\log \epsilon$ ) = 312 nm (4.25). IR (KBr,  $cm^{-1}$ ):  $\nu(O-H)$  3470 (*br*, C=N, thiazole), 1590 (*s*, C=N, azomethine), 1565 (*s*, C=O), 1360 (*m*, C–S–C), 760 (*m*);  $^1H$  NMR ( $d_6$ -DMSO, 200 MHz, p.p.m.): 13.30 (*s*, OH), 9.72 (*s*, 1H, CH=N), 6.95–7.99 (*m*, 7H), 3.65 (*s*, 3H). Analysis found: C 62.99, H 4.56, N 9.54%; calculated for  $C_{15}H_{12}N_2O_2S$ : C 63.38, H 4.23, N 9.86%;

### Crystal data

$C_{15}H_{12}N_2O_2S$

$M_r = 284.33$

Monoclinic,  $P2_1/n$

$a = 13.0117$  (12) Å

$b = 6.3408$  (4) Å

$c = 17.5237$  (15) Å

$\beta = 110.854$  (7)°

$V = 1351.07$  (19) Å<sup>3</sup>

$Z = 4$

$D_x = 1.398$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

Cell parameters from 9583

reflections

$\theta = 2.4$ – $29.3^\circ$

$\mu = 0.24$  mm<sup>-1</sup>

$T = 293$  (2) K

Block, red

$0.40 \times 0.38 \times 0.12$  mm

### Data collection

Stoe IPDS-2 diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: by

integration (*X-RED32*;

Stoe & Cie, 2002)

$T_{min} = 0.881$ ,  $T_{max} = 0.976$

9072 measured reflections

2642 independent reflections

1893 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.089$

$\theta_{max} = 26.0^\circ$

$h = -16 \rightarrow 16$

$k = -7 \rightarrow 7$

$l = -21 \rightarrow 21$

### Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.133$

$S = 0.95$

2642 reflections

181 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0793P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

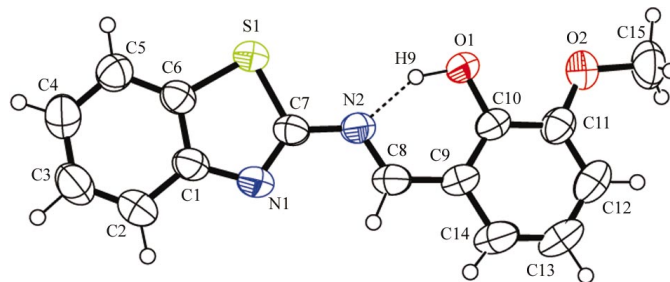
$\Delta\rho_{max} = 0.38$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.49$  e Å<sup>-3</sup>

**Table 1**

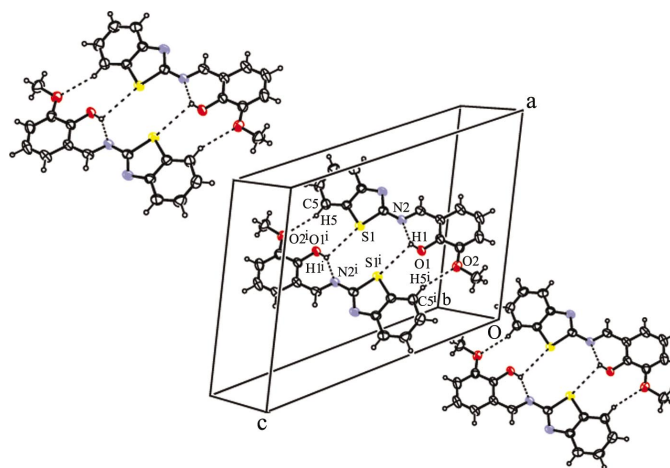
Selected geometric parameters (Å, °).

C1–N1	1.373 (3)	C8–N2	1.283 (3)
C6–S1	1.729 (2)	C10–O1	1.350 (2)
C7–N1	1.303 (3)	C11–O2	1.360 (3)
C7–N2	1.385 (3)	C15–O2	1.416 (3)
C7–S1	1.733 (2)		
N1–C7–N2	126.81 (19)	O2–C11–C12	125.5 (2)
N2–C7–S1	116.67 (14)	O2–C11–C10	114.85 (19)
O1–C10–C11	117.30 (19)	C8–N2–C7	119.80 (18)
O1–C10–C9	121.84 (19)		
N2–C8–C9–C10	−0.1 (4)	C5–C6–S1–C7	178.0 (2)
C14–C9–C10–O1	−178.3 (2)	C1–C6–S1–C7	−1.23 (18)
S1–C7–N1–C1	−0.7 (3)	N1–C7–S1–C6	1.19 (19)
S1–C7–N2–C8	171.46 (17)	N2–C7–S1–C6	−179.19 (18)



**Figure 1**

An ORTEP-3 (Farrugia, 1997) drawing of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The dashed line indicates the intramolecular hydrogen bond.



**Figure 2**

The hydrogen-bonding interactions (dashed lines) in (I) [symmetry code: (i)  $1 - x, 1 - y, 1 - z$ ].

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1–H1 $\cdots$ N2	0.82	1.87	2.593 (2)	147
C5–H5 $\cdots$ O2 <sup>i</sup>	0.93	2.51	3.395 (3)	160
O1–H1 $\cdots$ S1 <sup>i</sup>	0.82	2.97	3.1336 (14)	94

Symmetry code: (i)  $1 - x, 1 - y, 1 - z$ .

The hydroxy H atom was located in a difference Fourier map and the other H atoms were positioned geometrically. All H atoms were refined in the riding-model approximation, with O–H = 0.82 Å and C–H = 0.93–0.96 Å. For hydroxy and methyl H atoms,  $U_{iso}(H) = 1.5U_{eq}(C,O)$ ; for the other H atoms,  $U_{iso}(H) = 1.2U_{eq}(C)$ .

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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