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A monoclinic modification of 2-[(1,3-benzothiazol-2-yl)iminomethyl]phenol

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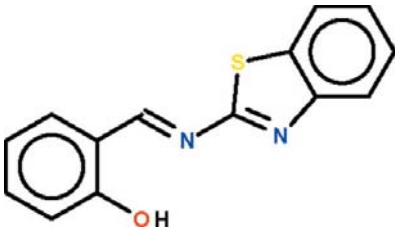
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.110; data-to-parameter ratio = 15.8.

In the title Schiff base, $C_{14}H_{10}N_2OS$, the azomethine double bond is in an E configuration; the benzothiazolyl ring (r.m.s. deviation = 0.007 Å) is coplanar with the phenylene ring (r.m.s. deviation = 0.007 Å), the two rings being slightly bent at 2.6 (1)°. The hydroxy H atom forms an intramolecular hydrogen bond to the imino group. The bond dimensions of the monoclinic modification are similar to those of the orthorhombic modification [Liu *et al.* (2009). *Acta Cryst.* E**65**, o738].

Related literature

For an orthorhombic modification of this structure, see: Liu *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{10}N_2OS$
M_r = 254.30
Monoclinic, Pn
a = 8.6391 (4) Å
b = 6.2313 (4) Å
c = 11.4459 (8) Å
β = 108.893 (1)°
V = 582.97 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 100 K
0.14 × 0.13 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.979
5307 measured reflections
2599 independent reflections
2512 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
S = 1.05
2599 reflections
164 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 1242 Friedel pairs
Flack parameter: 0.27 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.87	1.73	2.550 (2)	156

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2043).

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