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 /C27(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.110; data-to-parameter ratio = 15.8.

In the title Schiff base, C14H10N2OS, 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. E65, o738].

Related literature


Experimental

Crystal data

C14H10N2OS  M r = 254.30

Table 1

Hydrogen-bond geometry (Å, °).

D—H—A  D—H  H—A  D—A  D—H—A

O1—H1i···N1  0.87  1.73  2.55 (2)  156

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 > 2σ(I)
R int = 0.029

Reefinement

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

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

References