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4-Bromo-2-[(5-methylpyridin-2-ylimino)-methyl]phenol

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The molecule of the title compound, $C_{13}H_{11}BrN_2O$, displays a *trans* configuration with respect to the central C=N double bond and is almost planar. An intramolecular O—H···N hydrogen bond [O···N = 2.589 (6) Å] may influence the overall conformation.

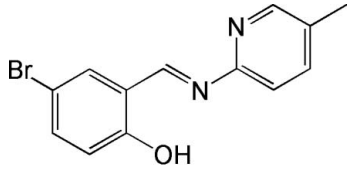
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.044
wR factor = 0.117
Data-to-parameter ratio = 15.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Schiff compounds play an important role in the development of coordination chemistry (Telfer *et al.*, 2004; Ramnauth *et al.*, 2004; Musie *et al.*, 2001; Bernardo *et al.*, 1996; Paul *et al.*, 2002). Two crystal structures of Schiff base compounds have recently been reported by the author (Yang, 2006*a*,*b*). As an extension of work on the structural characterization of such compounds, the crystal structure of the title compound, (I), is reported here (Fig. 1).



(I)

In (I), all the bond lengths are within normal ranges (Allen *et al.*, 1987) and comparable to the corresponding values observed in the similar crystal structures reported recently (Yang, 2006*a*), *e.g.* the central *trans* C7=N1 bond length of 1.269 (7) Å. The molecule is nearly planar, with a dihedral angle of 4.0 (5)° between the benzene ring and the pyridine ring. An intramolecular O—H···N hydrogen bond (Table 1) may influence the overall conformation. In the crystal structure, the molecular packing in (I) is stabilized only by van der

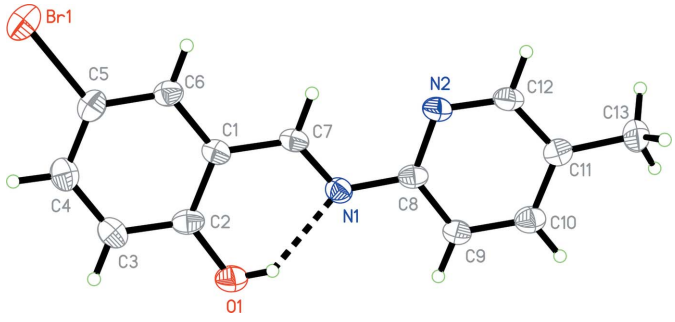


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

Waals interactions (Fig. 2) as there are no intermolecular hydrogen bonds or significant π–π stacking interactions.

Experimental

Reagents and solvents used were of commercially available quality. 5-Bromosalicylaldehyde (0.1 mmol, 20.1 mg) and 5-methyl-2-aminopyridine (0.1 mmol, 10.8 mg) were dissolved in MeOH (10 ml). The mixture was stirred at 298 K to give a clear yellow solution. Crystals of (I) were formed by slow evaporation of the solvent over a period of about 10 d at 298 K.

Crystal data

$C_{13}H_{11}BrN_2O$
M_r = 291.15
Orthorhombic, $Pna2_1$
a = 24.245 (4) Å
b = 4.358 (1) Å
c = 11.401 (2) Å
V = 1204.6 (4) Å^3
Z = 4
D_x = 1.605 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.40 mm^{-1}
T = 298 (2) K
Block, yellow
0.20 × 0.18 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.517, T_{max} = 0.545
8591 measured reflections
2456 independent reflections
1618 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.117
S = 1.07
2456 reflections
156 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 0.5825P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), 1141 Friedel pairs.
Flack parameter: 0.02 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.93	2.589 (6)	137

All H atoms were placed in idealized positions and constrained to ride on their parent atoms. Constrained distances: O—H = 0.82 Å, and C—H = 0.93 and 0.96 Å for methyl and aromatic CH groups, respectively. Isotropic displacement parameters were fixed at U_{iso}(H) = 1.2U_{iso}(C) for aromatic CH groups and 1.5U_{iso}(C,O) for other H atoms.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

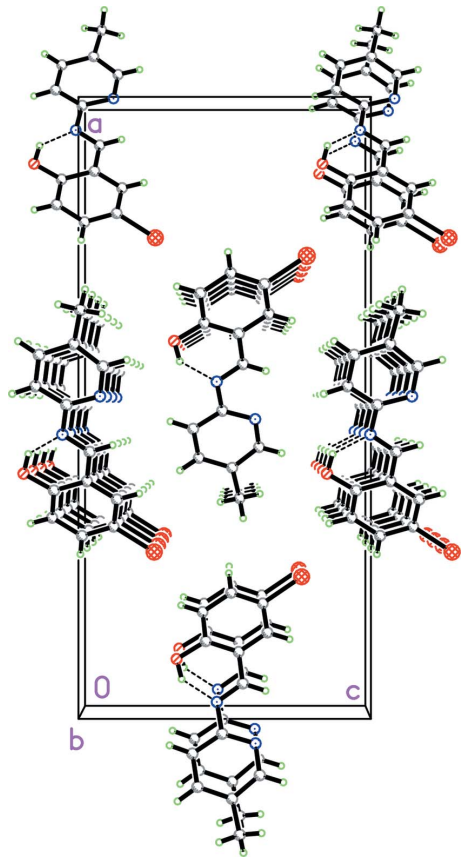


Figure 2
The crystal packing of (I). Dashed lines show the intramolecular hydrogen bonds.

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