2,4-Dibromo-6-(4-methylpyridin-2-ylimino-methyl)phenol

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Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.007 Å
R factor = 0.035
wR factor = 0.075
Data-to-parameter ratio = 15.8

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

The molecule of the title compound, $C_{13}H_{10}Br_2N_2O$, is nearly planar and displays a *trans* configuration with respect to the central C=N double bond. In the crystal structure, the molecules are linked through intermolecular C—H···Br hydrogen bonds, forming chains running along the b axis.

Comment

Schiff base compounds have been of great interest for a long time. These compounds have played an important role in the development of coordination chemistry (Bernardo *et al.*, 1996; Musie *et al.*, 2001; Paul *et al.*, 2002). 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)
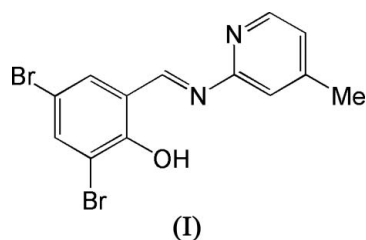
In compound (I), all the bond lengths are within normal ranges (Allen *et al.*, 1987), for example the central *trans* C7=N1 bond length of 1.265 (6) Å. The whole molecule is nearly planar, with a dihedral angle of 4.0 (4)° between the benzene ring and the pyridine ring. In the crystal structure, the molecules are linked through intermolecular C—H···Br hydrogen bonds (Table 1), forming chains running along the b axis (Fig. 2).

Experimental

3,5-Dibromosalicylaldehyde (0.1 mmol, 28.2 mg) and 2-amino-4-methylpyridine (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 one week at 298 K.

Crystal data

$C_{13}H_{10}Br_2N_2O$	$D_x = 1.869$ Mg m^{-3}
$M_r = 370.05$	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 1653
$a = 6.077$ (1) Å	reflections
$b = 14.224$ (2) Å	$\theta = 2.5$–24.1°
$c = 7.676$ (1) Å	$\mu = 6.15$ mm^{-1}
$\beta = 97.791$ (2)°	$T = 298$ (2) K
$V = 657.38$ (17) Å^3	Block, yellow
$Z = 2$	$0.20 \times 0.20 \times 0.19$ mm

Data collection

Bruker APEX area-detector
  diffractometer
ω scans
Absorption correction: multi-scan
  (*SADABS*; Bruker, 2002)
  $T_{min} = 0.298$, $T_{max} = 0.310$
5325 measured reflections

2617 independent reflections
2111 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 26.5°$
$h = -7 \rightarrow 7$
$k = -17 \rightarrow 17$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.075$
$S = 1.01$
2617 reflections
166 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983),
  1197 Freidel pairs
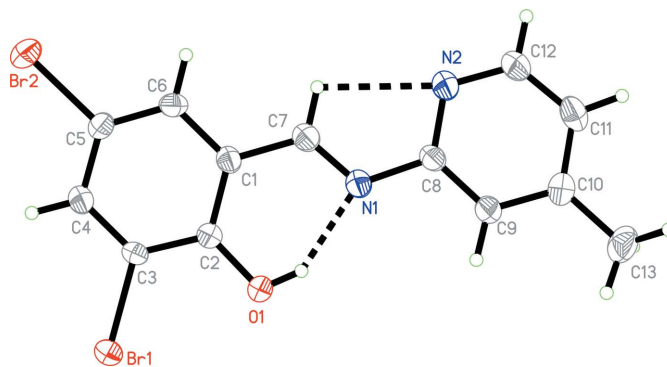Flack parameter: 0.389 (12)

Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines.
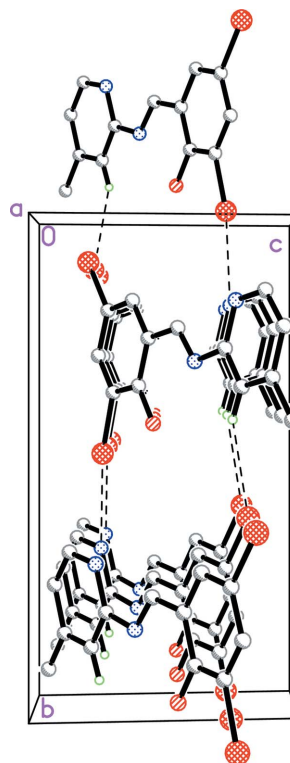
Table 1
Hydrogen-bond geometry (Å, °).

$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
C9—H9···Br2^i	0.93	2.92	3.783 (5)	155
O1—H1···N1	0.82	1.88	2.608 (5)	147
C7—H7···N2	0.93	2.32	2.698 (5)	104

Symmetry code: (i) $-x + 2, y + \frac{1}{2}, -z + 1$.

The refinement of the Flack (1983) parameter indicates partial inversion twinning. 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 CH$_3$ and aromatic CH groups, respectively. Isotropic displacement parameters were fixed at $U_{iso}(\mathrm{H}) = 1.2U_{iso}(\mathrm{C})$ for aromatic CH groups and $1.5U_{iso}(\mathrm{C,O})$ 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); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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Figure 2
The crystal packing of (I). Dashed lines show the intermolecular hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.