

to C6A, respectively, and by +1.8, +0.2, +2.8, -0.8, +0.3, and -0.4° on atoms C1B to C6B, respectively, with e.s.d.'s of approximately 0.2°.

The packing is shown in Fig. 2. With the van der Waals radii given by Nyburg & Faerman (1985) plus 1.70° Å as the radius for C, there are eight intermolecular distances shorter than the expected van der Waals distances, but only five of these involve a shortening of more than 0.1 Å. N1A is close to ring atoms in two different rings with an N1A...C4A distance of 3.158 (3) Å and an N1A...C5B distance of 3.104 (3) Å. N3A is in a similar situation but only the N3A...C6A distance of 3.184 (3) Å is short. The 1B nitrile group is more or less pointing towards a ring atom with an N1B...C4B distance of 3.089 (3) Å and a C11B—N1B...C4B angle of 141.9 (2)°. The 3B nitrile group also points toward a ring atom with an N3B...C2A distance of 3.083 (3) Å and a C33B—N3B...C2A angle of 160.9 (2)°.

Related literature. Structures of tetrafluorophthalonitrile (Britton, 1988), tetrafluoroterephthalonitrile

(Van Rij & Britton, 1981; Dunitz, Schweizer & Seiler, 1982; Seiler, Schweizer & Dunitz, 1984), and 5-chloro-2,4,6-trifluoroisophthalonitrile (Britton, 1991).

I thank Dr Robert Battershell for the sample of the compound.

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2-[(*o*-Hydroxyphenyl)imino]methylpyridine

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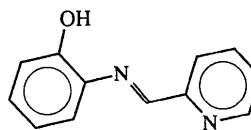
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Abstract. 2-[(2-Pyridylmethylene)amino]phenol, C₁₂H₁₀N₂O (1), *M_r* = 198.22, orthorhombic, *P*2₁2₁2₁, *a* = 4.722 (2), *b* = 12.284 (5), *c* = 17.638 (11) Å, *V* = 1023.0 (9) Å³, *Z* = 4, *D_x* = 1.29 Mg m⁻³, graphite-monochromated Mo *K*α radiation, λ = 0.71073 Å, μ = 0.08 mm⁻¹, *F*(000) = 416, *T* = 294 (1) K, *R* = 0.048 for 608 observed reflections. The relative planarity of the molecule (mean deviation = 0.049 Å) results in a close interaction between the proton at the *ortho* position of the phenyl ring [H(5)] and the proton of the imino group [H(6)]. This steric crowding is alleviated by expansion of the N(1)—C(6)—C(5) angle and by displacement of the two protons by 0.13 Å to opposite sides of the molecular plane. The *ortho*-hydroxy proton is involved in intramolecular hydrogen bonding to the imino N atom [H(1)...N(1) = 2.03 (8); O(1)...N(1) = 2.686 (7) Å; O(1)—H(1)...N(1) = 122 (7)°] and intermolecular

hydrogen bonding to the *ortho*-hydroxy O atom of an adjacent molecule [H(1)...O(1') = 2.30 (9); O(1)...O(1') = 2.987 (7) Å; O(1)—H(1)...O(1') = 126 (8)°]. The intermolecular hydrogen bonding links molecules into infinite chains; adjacent molecules in a chain are related by a 2₁ screw operation along the *a* axis.

Experimental. The title compound (1) was synthesized by literature methods (Pitt, Bao, Thompson, Wani, Rosenkrantz & Metterville, 1986). A yellow platey crystal, 0.05 × 0.40 × 0.60 mm, was used for data collection on a Nicolet R3m/V diffractometer,



(1)

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Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters ($\text{\AA}^2 \times 10^3$)

Equivalent isotropic U is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
O(1)	2961 (9)	3207 (4)	-162 (2)	70 (2)
N(1)	553 (9)	4228 (3)	1020 (2)	46 (2)
N(2)	-4096 (10)	4664 (4)	2563 (3)	58 (2)
C(1)	3789 (11)	4256 (5)	-6 (3)	49 (2)
C(2)	5799 (13)	4750 (6)	-469 (3)	64 (3)
C(3)	6653 (13)	5798 (6)	-327 (3)	62 (2)
C(4)	5501 (14)	6355 (6)	270 (3)	60 (2)
C(5)	3477 (13)	5882 (5)	725 (3)	57 (2)
C(6)	2579 (12)	4822 (4)	596 (3)	43 (2)
C(7)	-765 (12)	4665 (5)	1564 (3)	48 (2)
C(8)	-2873 (11)	4058 (5)	2018 (3)	48 (2)
C(9)	-3534 (14)	2981 (5)	1889 (4)	60 (2)
C(10)	-5524 (16)	2481 (7)	2353 (4)	71 (3)
C(11)	-6804 (15)	3106 (7)	2910 (4)	75 (3)
C(12)	-6059 (15)	4149 (8)	2989 (3)	73 (3)

with $\omega/2\theta$ scans of 2° min^{-1} , $3.5 \leq 2\theta \leq 45^\circ$, $h = 0$ to 6, $k = -14$ to 0, $l = 0$ to 20. 828 reflections were measured (all unique), of which 608 were observed [$I > 2.58\sigma(I)$]. Unit-cell dimensions were determined by least-squares fit to settings for 49 reflections ($26.34 < 2\theta < 36.78^\circ$). An empirical absorption correction was applied, transmission factors 0.85–1.00. Three standards (213, 127, 164) monitored over 13.9 h of X-ray exposure showed negligible ($\pm 2\%$) crystal decomposition. The structure was solved by direct methods; H atoms were located by standard difference Fourier techniques. Full-matrix least-squares refinement on F yielded $R = 0.0483$, $wR = 0.0569$, $S = 1.55$, $(\Delta/\sigma)_{\max} = 0.01$, for 177 variables including positional parameters, anisotropic thermal parameters for the non-H atoms, isotropic thermal parameters for H atoms and an isotropic extinction parameter [0.019 (3)]. The function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w = 1/\sigma^2(F_o)$; $\sigma(F_o)$ was estimated from counting statistics. Final difference Fourier peaks ranged from -0.16 to 0.21 e \AA^{-3} . Computations were performed using *SHELXTL* (Sheldrick, 1986). Scattering factors were those of Cromer & Waber (1974); real and imaginary anomalous-dispersion corrections were those of Cromer (1974). Final atomic coordinates are given in Table 1,* and bond distances and angles in Table 2; the molecule is displayed in Fig. 1.

Related literature. The thermochromic properties of (1) have been compared to salicylidene-2-amino-

* Lists of structure factors, H-atom coordinates, and distances and angles involving H atoms, anisotropic thermal parameters, best-planes data and torsion angles, and a packing diagram have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55121 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST0559]

Table 2. Bond distances (\AA) and angles ($^\circ$)

O(1)—C(1)	1.374 (7)	N(1)—C(6)	1.417 (7)
N(1)—C(7)	1.263 (7)	N(2)—C(8)	1.345 (7)
N(2)—C(12)	1.350 (9)	C(1)—C(2)	1.391 (8)
C(1)—C(6)	1.391 (7)	C(2)—C(3)	1.372 (11)
C(3)—C(4)	1.369 (9)	C(4)—C(5)	1.377 (9)
C(5)—C(6)	1.388 (8)	C(7)—C(8)	1.479 (8)
C(8)—C(9)	1.378 (8)	C(9)—C(10)	1.390 (10)
C(10)—C(11)	1.386 (11)	C(11)—C(12)	1.336 (13)
C(6)—N(1)—C(7)	121.1 (5)	C(8)—N(2)—C(12)	115.7 (5)
O(1)—C(1)—C(2)	119.0 (5)	O(1)—C(1)—C(6)	120.3 (5)
C(2)—C(1)—C(6)	120.7 (6)	C(1)—C(2)—C(3)	120.1 (6)
C(2)—C(3)—C(4)	119.5 (6)	C(3)—C(4)—C(5)	120.9 (6)
C(4)—C(5)—C(6)	120.8 (6)	N(1)—C(6)—C(1)	115.1 (5)
N(1)—C(6)—C(5)	127.0 (5)	C(1)—C(6)—C(5)	117.9 (5)
N(1)—C(7)—C(8)	121.9 (5)	N(2)—C(8)—C(7)	113.4 (5)
N(2)—C(8)—C(9)	123.5 (5)	C(7)—C(8)—C(9)	123.1 (5)
C(8)—C(9)—C(10)	118.7 (6)	C(9)—C(10)—C(11)	117.9 (7)
C(10)—C(11)—C(12)	119.4 (7)	N(2)—C(12)—C(11)	124.9 (7)

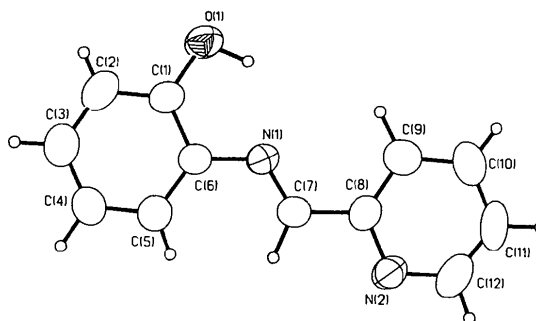


Fig. 1. Molecular structure and numbering scheme, thermal ellipsoids at 50% probability level. H atoms have arbitrary radii.

pyridines (Hadjoudis, Moustakali-Mavridis & Xexakis, 1979). Structural data were reported for the latter compounds only. Compound (1) and related imines have found extensive use as analytical reagents [for a representative example see Otomo & Kodama (1973)].

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