Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[(Pyridin-3-ylamino)methyl]phenol

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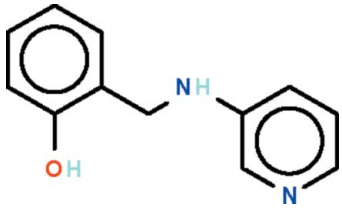
Received 4 November 2011; accepted 7 November 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.137; data-to-parameter ratio = 16.4.

In the title compound, $C_{12}H_{12}N_2O$, the aromatic rings at either ends of the –CH_2–NH– link are twisted by 68.79 (7)°. In the crystal, the hydroxy substituent is a hydrogen-bond donor to the N atom of the pyridine ring of an adjacent molecule, and the hydrogen bond generates a chain along the b axis; it is also a hydrogen-bond acceptor to the amino group of another adjacent molecule. The two hydrogen bonds lead to the formation of a layer structure.

Related literature

For the *N*-salicylidene-3-aminopyridine precursor, see: Csaszar (1990); Kaya & Guelel (2005); Robert *et al.* (2009). For a related structure, see: Xu *et al.* (2011).



Experimental

Crystal data

$C_{12}H_{12}N_2O$
M_r = 200.24
Monoclinic, $P2_1/c$
a = 5.8386 (11) Å
b = 13.399 (3) Å
c = 13.169 (3) Å
β = 90.519 (6)°
V = 1030.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.21 × 0.12 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.983, T_{max} = 0.990
9845 measured reflections
2358 independent reflections
1879 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.137
S = 1.08
2358 reflections
144 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···N2^{i}	0.86 (1)	1.80 (1)	2.6568 (16)	175 (2)
N1—H1n···O1^{ii}	0.88 (1)	2.38 (1)	3.2296 (17)	163 (1)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); 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).

This work was supported by the Key Project of the Natural Science Foundation of Heilongjiang Province (No. ZD200903), the Key Project of the Education Bureau of Heilongjiang Province (No. 12511z023), Heilongjiang University (Hdtd2010–04) and the University of Malaya.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5384).

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supporting information

Acta Cryst. (2011). E**67**, o3259 [https://doi.org/10.1107/S160053681104685X]

2-[(Pyridin-3-ylamino)methyl]phenol

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S1. Comment

There are numerous studies on the Schiff bases derived by condensing salicyldehyde and an aromatic amine. In this study, the azomethine double-bond of *N*-salicylidene-3-aminopyridine (Csaszar, 1990; Kaya & Guelel, 2005; Robert *et al.* 2009) is reduced by sodium borohydride to yield the title secondary amine (Scheme I). The two aromatic rings at either ends of the $–CH_2–NH–$ link of $C_{12}H_{12}N_2O$ are twisted by 68.79 (7)° (Fig. 1). The hydroxy substituent is hydrogen-bond donor to the N atom of the pyridyl ring of an adjacent molecule, and the hydrogen bond generates a linear chain along the *b*-axis. It is also hydrogen-bond acceptor to the amino group of another adjacent molecule; the two hydrogen bonds lead to the formation of a layer structure (Table 1).

S2. Experimental

A solution of 3-aminopyridine (1 mmol) and salicylaldehyde (1 mmol) in toluene (50 ml) was heated for 10 h. The solvent was removed under vacuum, and the residue was reduced in absolute methanol by sodium borohydride. Colorless crystals were obtained by recrystallization from methanol; yield 80%.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C). The amino and hydroxy H-atoms were located in a difference Fourier map, and were refined with distance restraints N–H 0.88±0.01 Å and O–H 0.84±0.01 Å; their temperature factors were refined.

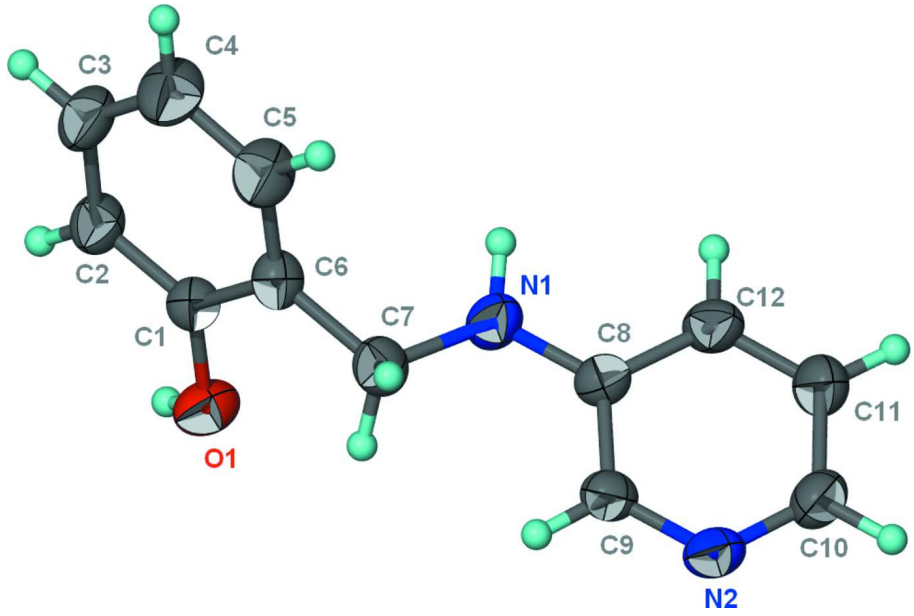

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{12}H_{12}N_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-[(Pyridin-3-ylamino)methyl]phenol

Crystal data

$C_{12}H_{12}N_2O$
$M_r = 200.24$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.8386$ (11) Å
$b = 13.399$ (3) Å
$c = 13.169$ (3) Å
$\beta = 90.519$ (6)°
$V = 1030.1$ (4) Å^3
$Z = 4$

$F(000) = 424$
$D_x = 1.291$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5377 reflections
$\theta = 3.0$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Prism, colorless
0.21 × 0.12 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.983$, $T_{max} = 0.990$

9845 measured reflections
2358 independent reflections
1879 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -7 \rightarrow 7$
$k = -17 \rightarrow 17$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.137$
$S = 1.08$

2358 reflections
144 parameters
2 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2 + 0.0952P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.17862 (17)	0.30493 (7)	0.38420 (7)	0.0517 (3)
H1O	1.249 (3)	0.2486 (9)	0.3790 (12)	0.073 (5)*
N1	0.6391 (2)	0.42170 (9)	0.32008 (9)	0.0512 (3)
H1N	0.534 (2)	0.3813 (10)	0.3444 (11)	0.059 (4)*
N2	0.61025 (18)	0.63154 (8)	0.14353 (8)	0.0493 (3)
C1	1.0374 (2)	0.30367 (9)	0.46539 (9)	0.0396 (3)
C2	1.0673 (2)	0.23629 (11)	0.54458 (10)	0.0499 (3)
H2	1.1882	0.1911	0.5429	0.060*
C3	0.9202 (3)	0.23577 (13)	0.62516 (10)	0.0591 (4)
H3	0.9407	0.1897	0.6773	0.071*
C4	0.7428 (3)	0.30289 (14)	0.62928 (11)	0.0669 (5)
H4	0.6418	0.3022	0.6835	0.080*
C5	0.7166 (3)	0.37110 (12)	0.55208 (11)	0.0597 (4)
H5	0.5982	0.4173	0.5557	0.072*
C6	0.8605 (2)	0.37334 (9)	0.46929 (9)	0.0431 (3)
C7	0.8270 (2)	0.44915 (10)	0.38681 (11)	0.0484 (3)
H7A	0.7961	0.5138	0.4169	0.058*
H7B	0.9664	0.4547	0.3477	0.058*
C8	0.5640 (2)	0.48446 (9)	0.24474 (9)	0.0416 (3)
C9	0.6833 (2)	0.57012 (10)	0.21638 (10)	0.0449 (3)
H9	0.8200	0.5850	0.2499	0.054*
C10	0.4163 (2)	0.61131 (11)	0.09441 (11)	0.0545 (4)
H10	0.3659	0.6543	0.0434	0.065*
C11	0.2877 (2)	0.52808 (12)	0.11717 (11)	0.0586 (4)
H11	0.1522	0.5152	0.0819	0.070*
C12	0.3611 (2)	0.46471 (11)	0.19197 (10)	0.0528 (4)
H12	0.2755	0.4083	0.2077	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0596 (6)	0.0440 (5)	0.0517 (6)	0.0094 (4)	0.0165 (5)	0.0042 (4)
N1	0.0588 (7)	0.0428 (6)	0.0519 (6)	−0.0104 (5)	−0.0083 (5)	0.0094 (5)
N2	0.0515 (6)	0.0442 (6)	0.0522 (6)	−0.0019 (5)	0.0093 (5)	0.0090 (5)
C1	0.0424 (6)	0.0385 (6)	0.0380 (6)	0.0015 (5)	0.0016 (5)	−0.0046 (5)
C2	0.0494 (7)	0.0527 (8)	0.0476 (7)	0.0131 (6)	0.0022 (6)	0.0037 (6)
C3	0.0645 (9)	0.0721 (10)	0.0408 (7)	0.0146 (7)	0.0030 (6)	0.0107 (6)
C4	0.0663 (9)	0.0880 (12)	0.0467 (8)	0.0213 (8)	0.0168 (7)	0.0033 (7)
C5	0.0570 (8)	0.0670 (10)	0.0551 (8)	0.0241 (7)	0.0097 (7)	−0.0013 (7)

C6	0.0448 (6)	0.0413 (7)	0.0432 (6)	0.0053 (5)	−0.0032 (5)	−0.0040 (5)
C7	0.0465 (7)	0.0396 (7)	0.0589 (8)	0.0025 (5)	−0.0045 (6)	0.0019 (6)
C8	0.0473 (6)	0.0377 (6)	0.0400 (6)	−0.0011 (5)	0.0038 (5)	−0.0009 (5)
C9	0.0403 (6)	0.0434 (7)	0.0511 (7)	−0.0022 (5)	0.0045 (5)	0.0029 (5)
C10	0.0592 (8)	0.0578 (8)	0.0465 (7)	0.0034 (6)	0.0008 (6)	0.0120 (6)
C11	0.0558 (8)	0.0701 (10)	0.0498 (8)	−0.0095 (7)	−0.0094 (6)	0.0057 (7)
C12	0.0584 (8)	0.0518 (8)	0.0481 (7)	−0.0169 (6)	−0.0026 (6)	0.0037 (6)

Geometric parameters (Å, º)

O1—C1	1.3562 (15)	C4—H4	0.9300
O1—H1O	0.86 (1)	C5—C6	1.383 (2)
N1—C8	1.3695 (16)	C5—H5	0.9300
N1—C7	1.4472 (17)	C6—C7	1.4986 (17)
N1—H1N	0.88 (1)	C7—H7A	0.9700
N2—C10	1.3269 (18)	C7—H7B	0.9700
N2—C9	1.3312 (16)	C8—C12	1.3936 (18)
C1—C2	1.3892 (18)	C8—C9	1.3953 (18)
C1—C6	1.3933 (17)	C9—H9	0.9300
C2—C3	1.371 (2)	C10—C11	1.379 (2)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.373 (2)	C11—C12	1.366 (2)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.374 (2)	C12—H12	0.9300
C1—O1—H1O	110.3 (12)	C1—C6—C7	121.29 (12)
C8—N1—C7	121.31 (11)	N1—C7—C6	111.17 (11)
C8—N1—H1N	114.9 (10)	N1—C7—H7A	109.4
C7—N1—H1N	117.6 (10)	C6—C7—H7A	109.4
C10—N2—C9	119.43 (11)	N1—C7—H7B	109.4
O1—C1—C2	121.78 (11)	C6—C7—H7B	109.4
O1—C1—C6	118.47 (11)	H7A—C7—H7B	108.0
C2—C1—C6	119.73 (12)	N1—C8—C12	120.65 (11)
C3—C2—C1	120.58 (12)	N1—C8—C9	122.81 (11)
C3—C2—H2	119.7	C12—C8—C9	116.54 (12)
C1—C2—H2	119.7	N2—C9—C8	122.96 (12)
C2—C3—C4	120.35 (13)	N2—C9—H9	118.5
C2—C3—H3	119.8	C8—C9—H9	118.5
C4—C3—H3	119.8	N2—C10—C11	121.55 (12)
C3—C4—C5	119.01 (14)	N2—C10—H10	119.2
C3—C4—H4	120.5	C11—C10—H10	119.2
C5—C4—H4	120.5	C12—C11—C10	119.44 (13)
C4—C5—C6	122.24 (13)	C12—C11—H11	120.3
C4—C5—H5	118.9	C10—C11—H11	120.3
C6—C5—H5	118.9	C11—C12—C8	120.07 (12)
C5—C6—C1	118.05 (12)	C11—C12—H12	120.0
C5—C6—C7	120.66 (11)	C8—C12—H12	120.0

O1—C1—C2—C3	−179.14 (13)	C5—C6—C7—N1	−77.50 (16)
C6—C1—C2—C3	1.9 (2)	C1—C6—C7—N1	102.91 (14)
C1—C2—C3—C4	−0.9 (2)	C7—N1—C8—C12	−169.54 (13)
C2—C3—C4—C5	−0.7 (3)	C7—N1—C8—C9	10.6 (2)
C3—C4—C5—C6	1.2 (3)	C10—N2—C9—C8	−0.4 (2)
C4—C5—C6—C1	−0.2 (2)	N1—C8—C9—N2	−179.66 (12)
C4—C5—C6—C7	−179.76 (14)	C12—C8—C9—N2	0.5 (2)
O1—C1—C6—C5	179.63 (12)	C9—N2—C10—C11	0.2 (2)
C2—C1—C6—C5	−1.41 (19)	N2—C10—C11—C12	0.0 (2)
O1—C1—C6—C7	−0.77 (17)	C10—C11—C12—C8	0.1 (2)
C2—C1—C6—C7	178.19 (11)	N1—C8—C12—C11	179.81 (14)
C8—N1—C7—C6	174.01 (12)	C9—C8—C12—C11	−0.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1o···N2^{i}	0.86 (1)	1.80 (1)	2.6568 (16)	175 (2)
N1—H1n···O1^{ii}	0.88 (1)	2.38 (1)	3.2296 (17)	163 (1)

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+1/2; (ii) *x*−1, *y*, *z*.