Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Bromo-2-(2-pyridylmethyliminomethyl)phenol

Yiqun Zhang,[a] Lian Ee Khoo[a] and Seik Weng Ng[b]*

[a]National Institute of Education, Nanyang Technological Univerity, Singapore, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.045
wR factor = 0.108
Data-to-parameter ratio = 13.3

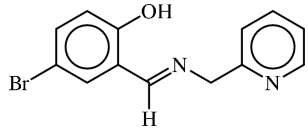
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 5 September 2003
Accepted 9 September 2003
Online 18 September 2003

Two molecules of the title compound, $C_{13}H_{11}BrN_2O$, are linked by an intermolecular $Br\cdots N_{pyridyl}$ interaction of 3.263 (4) Å across a center of inversion. The imino N atom is engaged in intramolecular hydrogen bonding with the phenol group [$O\cdots N$ = 2.595 (5) Å].

Comment

Schiff bases derived from the condensation of salicylaldehyde and a primary amine can be further reduced by sodium borohydride to form substituted phenol derivatives having both secondary and tertiary amino groups on the same substituent, *e.g.* 2-OH-4-NO_2-3-CH_2-NH-CH_2CH_2-N$(CH_3)_2$, which, owing to its existence in the zwitterionic form (Hazell *et al.*, 1997), is an excellent Lewis base that can coordinate to organotin Lewis acids. With the less electron-withdrawing Br atom in place of the $-NO_2$ group, the compound probably does not exist in this zwitterionic form. However, the molecule is able to form complexes (Khoo, Yan, Goh & Ng, 2000; Khoo *et al.*, 2001). A previous study on the Schiff base 7-methoxy-3-(salicyldene)aminocoumarin (Khoo, Zhang & Ng, 2000) has revealed potentially useful lasing activity.



(I)

The bromo-substituted title compound, (I), is a monomeric compound whose hydroxy group is engaged in hydrogen bonding with the imino N atom (Fig. 1). Two molecules are linked by a $Br\cdots N_{pyridyl}$ interaction across an inversion center, forming a dimeric entity (Fig. 2).

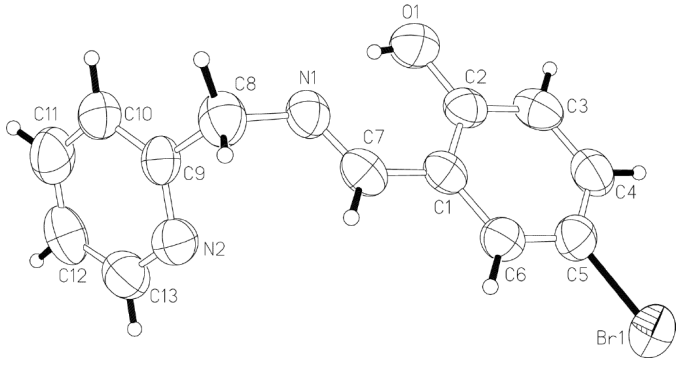


Figure 1
ORTEP plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

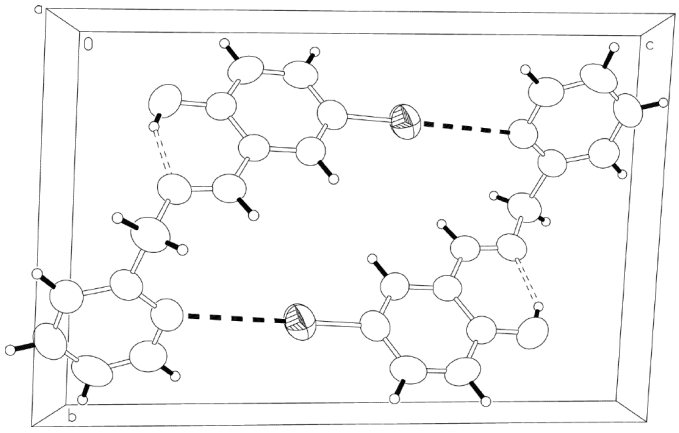


Figure 2
ORTEP plot of the Br···N-linked dimeric unit.

Experimental

The compound was synthesized by condensing equimolar quantities of 5-bromosalicylaldehyde and 2-(aminomethyl)pyridine in chloroform, duplicating the method used for the synthesis of 2-(3-pyridylmethyliminomethyl)phenol (Cimerman *et al.*, 1994).

Crystal data

$C_{13}H_{11}BrN_2O$
M_r = 291.15
Triclinic, $P\overline{1}$
a = 4.474 (1) Å
b = 9.529 (2) Å
c = 14.271 (2) Å
α = 92.65 (1)°
β = 93.72 (1)°
γ = 95.16 (2)°
V = 603.8 (2) Å^3
Z = 2
D_x = 1.601 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 4.5–12.7°
μ = 3.39 mm^{-1}
T = 298 (2) K
Block, yellow
0.20 × 0.20 × 0.10 mm

Data collection

Siemens $P4$ four-circle diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.531, T_{max} = 0.713
2912 measured reflections
2069 independent reflections
1416 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°
$h = -5 \rightarrow 1$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 16$
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.108
S = 1.01
2069 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.2428P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C5	1.901 (4)	C2—C3	1.395 (6)
O1—C2	1.343 (5)	C3—C4	1.379 (6)
N1—C7	1.269 (5)	C4—C5	1.384 (6)
N1—C8	1.458 (6)	C5—C6	1.370 (6)
N2—C9	1.330 (5)	C8—C9	1.513 (6)
N2—C13	1.319 (6)	C9—C10	1.371 (6)
C1—C2	1.396 (6)	C10—C11	1.377 (7)
C1—C6	1.385 (6)	C11—C12	1.361 (8)
C1—C7	1.461 (6)	C12—C13	1.361 (7)
C7—N1—C8	118.3 (4)	C6—C5—Br1	120.4 (3)
C9—N2—C13	116.9 (4)	C5—C6—C1	120.7 (4)
C6—C1—C2	119.1 (4)	N1—C7—C1	122.2 (4)
C6—C1—C7	120.1 (4)	N1—C8—C9	109.9 (4)
C2—C1—C7	120.8 (4)	N2—C9—C8	115.0 (4)
O1—C2—C1	121.8 (4)	N2—C9—C10	122.5 (4)
O1—C2—C3	118.5 (4)	C10—C9—C8	122.5 (4)
C1—C2—C3	119.6 (4)	C9—C10—C11	119.0 (5)
C2—C3—C4	120.5 (4)	C12—C11—C10	118.7 (5)
C3—C4—C5	119.2 (4)	C11—C12—C13	118.1 (5)
C4—C5—C6	120.8 (4)	N2—C13—C12	124.7 (5)
C4—C5—Br1	118.8 (3)		

H atoms were positioned geometrically (C—H = 0.93 Å for sp^2-hybridized C atoms, C—H = 0.97 Å for the sp^3-hybridized C atom and O—H = 0.82 Å for the phenol H atom). Displacement parameters were set to $1.2U_{eq}$ of the parent atoms for the aromatic H atoms and $1.5U_{eq}$ for the other H atoms.

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *LEAST SQUARES* in *XSCANS*; data reduction: *REDUCE* in *XSCANS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

The authors thank Nanyang Technological University and the University of Malaya for supporting this work.

References

Bruker (1997). *XSCANS*. Version 2.21. Bruker AXS Inc., Madison, Wisconsin, USA.
Cimerman, Z., Kiralj, R. & Galić, N. (1994). *J. Mol. Struct.* **323**, 7–14.
Hazell, A., Overgaard, J., Lausen, S. K., Hu, H. & Khoo, L. E. (1997). *Acta Cryst.* C**53**, 640–641.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Khoo, L. E., Yan, B., Goh, N. K. & Ng, S. W. (2000). *Main Group Met. Chem.* **23**, 721–722.
Khoo, L. E., Yan, B., Goh, N. K. & Ng, S. W. (2001). *Main Group Met. Chem.* **24**, 817–818.
Khoo, L. E., Zhang, Y. & Ng, S. W. (2000). *Acta Cryst.* C**56**, e350–e351.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.