Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-4-Bromo-2-[(4-ethylphenyl)iminomethyl]phenol

Şehriman Atalay,[a]* Talip Kaya Erdem,[a] Ferda Erşahin[b] and Nihat Tınkılıç[b]

[a]Department of Physics, Ondokuz Mayıs University, TR-55139 Samsun, Turkey, and [b]Department of Chemistry, Ondokuz Mayıs University, TR-55139 Samsun, Turkey
Correspondence e-mail: atalays@omu.edu.tr

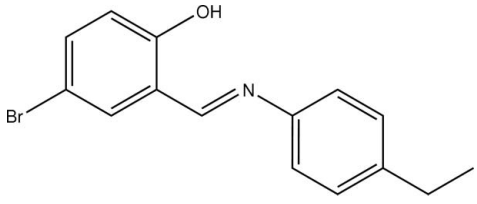
Received 5 November 2007; accepted 13 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.014 Å; R factor = 0.041; wR factor = 0.109; data-to-parameter ratio = 8.0.

In the title compound, $C_{15}H_{14}BrNO$, the dihedral angle between the two benzene rings is 43.99 (2)°. The molecular conformation is influenced by an intramolecular O—H···N hydrogen bond.

Related literature

For related literature, see: Akkaya *et al.* (2007); Atalay *et al.* (2005, 2006); Calligaris & Randaccio (1987).



Experimental

Crystal data

$C_{15}H_{14}BrNO$
M_r = 304.18
Orthorhombic, $Pna2_1$
a = 6.2280 (6) Å
b = 7.0292 (7) Å
c = 30.237 (4) Å
V = 1323.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.09 mm^{-1}
T = 293 (2) K
0.48 × 0.31 × 0.05 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.521, T_{max} = 0.809
7324 measured reflections
1318 independent reflections
819 reflections with $I > 2\sigma(I)$
R_{int} = 0.102

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.109
S = 0.92
1318 reflections
165 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Absolute structure: Flack (1983), with 1231 Friedel pairs
Flack parameter: 0.10 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.89	2.609 (10)	146

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

The authors thank the Turkish Goverment and the University of Ondokuz Mayıs for research grant F443.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2219).

References

Akkaya, A., Erşahin, F., Şenel, I., Ağar, E. & Büyükgüngör, O. (2007). *Acta Cryst.* E**63**, o2383–o2385.
Atalay, S., Ocak İskeleli, N., Ağar, E. & Akdemir, N (2005). *Acta Cryst.* E**61**, o2654–o2655.
Atalay, Ş., Petek, H., Ocak İskeleli, N., Albayrak, Ç. & Ağar, E. (2006). *Acta Cryst.* E**62**, o3092–o3093.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Calligaris, M. & Randaccio, L. (1987). *Comprehensive Coordination Chemistry*, Vol. 2, edited by G. Wilkinson, pp. 715–738. London: Pergamon.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.118) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.

  doi:10.1107/S1600536807058618

supporting information

Acta Cryst. (2008). E**64**, o92 [https://doi.org/10.1107/S1600536807058618]

(*E*)-4-Bromo-2-[(4-ethylphenyl)iminomethyl]phenol

Şehriman Atalay, Talip Kaya Erdem, Ferda Erşahin and Nihat Tınkılıç

S1. Comment

Schiff bases exhibit biological activity and they are widely used as ligands in metal complexes (Calligaris & Randaccio 1987).

In the title compound the dihedral angle between the benzene rings rings is 43.99 (2)°. The N?C and N—C bond lengths, 1.264 (10) Å and 1.417 (10) Å, respectively, agree with literature values (Akkaya *et al.*, 2007; Atalay *et al.*, 2006). The Br1—C4 and C1—O1 bond lengths are 1.878 (9) Å and 1.371 (12) Å, respectively, in good agreement with the literature (Atalay *et al.*, 2005). The molecular conformation is influenced by an O—H···N hydrogen bond (Table 1, Fig. 1).

S2. Experimental

The title compound, (*E*)-2-[(4-ethylphenylimino)methyl]-4-bromophenol, was prepared by refluxing a mixture of a solution containing 5-bromosalicylaldehyde (0.05 ml, 0.25 mmol) in 20 ml e thanol and a solution containing 4-ethyl-aniline (0.03 g, 0.25 mmol) in 20 ml e thanol. The reaction mixture was stirred for 1 h under reflux. Crystals of the title compound suitable for X-ray analysis were obtained from an acetonitrile solution by slow evaporation (yield 84%; m.p. 385–386 K).

S3. Refinement

All H atoms were placed in calculated positions and refined using a riding model, with aromatic C—H = 0.93 Å for Csp^2, 0.97 Å for methylene and 0.96 Å for methyl; O—H = 0.82 Å. U_{iso}(H) = xU_{eq}(carrier atom), where x = 1.5 for O and 1.2 for all C atoms. The value of R_{int} is rather high because of the poor data quality.

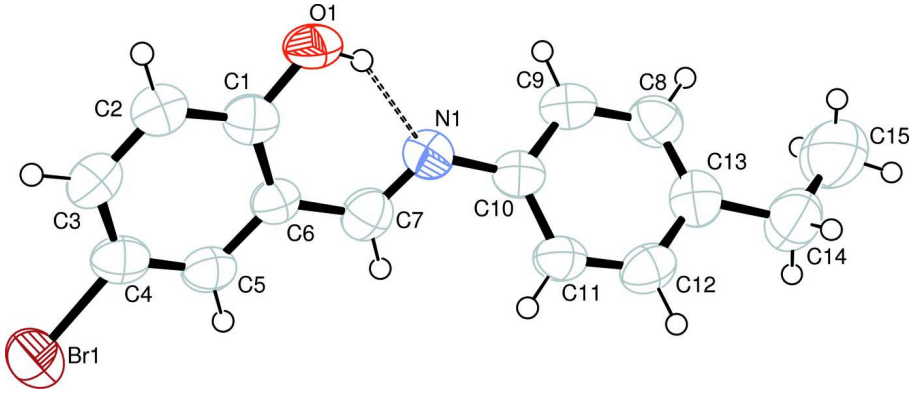


Figure 1

The molecular structure of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids. The hydrogen bond is shown as a double-dashed line.

(*E*)-4-Bromo-2-[(4-ethylphenyl)iminomethyl]phenol

Crystal data

$C_{15}H_{14}BrNO$
$M_r = 304.18$
Orthorhombic, $Pna2_1$
$a = 6.2280$ (6) Å
$b = 7.0292$ (7) Å
$c = 30.237$ (4) Å
$V = 1323.7$ (3) Å^3
$Z = 4$
$F(000) = 616$
$D_x = 1.526$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9683 reflections
$\theta = 1.4$–$26.1°$
$\mu = 3.09$ mm^{-1}
$T = 293$ K
Plate, yellow
0.48 × 0.31 × 0.05 mm

Data collection

STOE IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
w scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.521$, $T_{max} = 0.809$
7324 measured reflections
1318 independent reflections
819 reflections with $I > 2\sigma(I)$
$R_{int} = 0.102$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.4°$
$h = -7 \rightarrow 7$
$k = -8 \rightarrow 8$
$l = -36 \rightarrow 36$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.109$
$S = 0.92$
1318 reflections
165 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0011 (7)
Absolute structure: Flack (1983), 1231 Friedel pairs
Absolute structure parameter: 0.10 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C7	0.6103 (14)	0.4481 (11)	0.6165 (3)	0.0602 (19)

H7	0.7542	0.4132	0.6152	0.072*
C5	0.6251 (12)	0.4361 (11)	0.6979 (3)	0.0562 (18)
H5	0.7652	0.3907	0.6964	0.067*
C3	0.3255 (13)	0.5382 (12)	0.7420 (3)	0.063 (2)
H3	0.2663	0.5628	0.7697	0.076*
C12	0.9101 (13)	0.5783 (11)	0.4937 (3)	0.063 (2)
H12	1.0455	0.6323	0.4904	0.075*
C1	0.2969 (13)	0.5335 (10)	0.6631 (3)	0.0576 (18)
C4	0.5322 (13)	0.4707 (12)	0.7385 (3)	0.0582 (19)
C11	0.8254 (11)	0.5622 (12)	0.5348 (3)	0.0578 (19)
H11	0.9024	0.6024	0.5594	0.069*
C6	0.5101 (12)	0.4686 (10)	0.6591 (2)	0.0512 (16)
C9	0.5119 (15)	0.4235 (12)	0.5023 (3)	0.061 (2)
H9	0.3741	0.3737	0.5048	0.073*
C8	0.6088 (16)	0.4367 (13)	0.4610 (3)	0.066 (2)
H8	0.5380	0.3889	0.4363	0.079*
C13	0.8010 (18)	0.5166 (17)	0.4562 (4)	0.067 (3)
C14	0.9191 (18)	0.5424 (16)	0.4110 (4)	0.092 (3)
H14A	0.9304	0.6775	0.4049	0.111*
H14B	1.0639	0.4932	0.4140	0.111*
C2	0.2089 (15)	0.5685 (12)	0.7048 (5)	0.057 (3)
H2	0.0688	0.6131	0.7070	0.069*
C10	0.6197 (12)	0.4841 (10)	0.5396 (2)	0.0523 (18)
C15	0.819 (3)	0.451 (3)	0.3735 (8)	0.141 (9)
H15A	0.8126	0.3164	0.3784	0.169*
H15B	0.9021	0.4763	0.3473	0.169*
H15C	0.6765	0.5002	0.3697	0.169*
N1	0.5106 (11)	0.4758 (10)	0.5806 (2)	0.0553 (18)
O1	0.1708 (9)	0.5649 (9)	0.6266 (3)	0.067 (2)
H1	0.2389	0.5395	0.6042	0.100*
Br1	0.70006 (13)	0.43768 (13)	0.78954 (7)	0.0838 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C7	0.063 (4)	0.051 (5)	0.067 (5)	−0.009 (4)	0.004 (4)	−0.001 (4)
C5	0.047 (4)	0.051 (5)	0.070 (5)	−0.007 (3)	−0.004 (4)	0.003 (4)
C3	0.054 (5)	0.063 (5)	0.073 (5)	0.001 (4)	0.013 (4)	0.002 (4)
C12	0.056 (4)	0.048 (5)	0.084 (6)	−0.005 (4)	0.003 (4)	0.004 (4)
C1	0.057 (4)	0.049 (4)	0.067 (4)	−0.002 (4)	−0.005 (4)	−0.002 (4)
C4	0.054 (4)	0.045 (5)	0.076 (5)	−0.007 (3)	−0.007 (4)	−0.001 (4)
C11	0.051 (5)	0.054 (5)	0.069 (5)	−0.005 (4)	−0.010 (4)	0.003 (4)
C6	0.044 (4)	0.052 (4)	0.058 (4)	0.001 (3)	0.001 (3)	0.001 (4)
C9	0.050 (5)	0.057 (6)	0.075 (5)	0.000 (4)	−0.004 (4)	−0.008 (4)
C8	0.071 (5)	0.061 (6)	0.066 (5)	−0.007 (5)	−0.008 (4)	−0.007 (4)
C13	0.073 (6)	0.061 (6)	0.066 (6)	0.009 (5)	0.005 (5)	−0.001 (5)
C14	0.090 (7)	0.102 (8)	0.086 (6)	−0.015 (6)	0.017 (6)	−0.001 (7)
C2	0.053 (5)	0.049 (5)	0.070 (7)	0.002 (4)	0.001 (5)	0.001 (5)

C10	0.050 (4)	0.044 (5)	0.063 (4)	0.008 (3)	−0.002 (4)	−0.004 (4)
C15	0.112 (13)	0.22 (2)	0.094 (15)	−0.025 (11)	0.020 (10)	−0.015 (12)
N1	0.056 (4)	0.054 (5)	0.056 (4)	0.004 (4)	−0.003 (3)	−0.003 (4)
O1	0.040 (3)	0.089 (5)	0.073 (4)	0.009 (3)	−0.005 (3)	−0.002 (4)
Br1	0.0808 (5)	0.1063 (7)	0.0642 (4)	0.0050 (5)	−0.0098 (8)	−0.0008 (10)

Geometric parameters (Å, º)

C7—N1	1.264 (10)	C11—H11	0.9300
C7—C6	1.440 (11)	C9—C10	1.378 (11)
C7—H7	0.9300	C9—C8	1.391 (12)
C5—C4	1.379 (12)	C9—H9	0.9300
C5—C6	1.394 (11)	C8—C13	1.330 (14)
C5—H5	0.9300	C8—H8	0.9300
C3—C2	1.357 (18)	C13—C14	1.562 (15)
C3—C4	1.376 (12)	C14—C15	1.45 (2)
C3—H3	0.9300	C14—H14A	0.9700
C12—C11	1.356 (11)	C14—H14B	0.9700
C12—C13	1.390 (14)	C2—H2	0.9300
C12—H12	0.9300	C10—N1	1.417 (10)
C1—O1	1.371 (12)	C15—H15A	0.9600
C1—C2	1.397 (17)	C15—H15B	0.9600
C1—C6	1.409 (10)	C15—H15C	0.9600
C4—Br1	1.878 (9)	O1—H1	0.8200
C11—C10	1.401 (10)		
N1—C7—C6	122.6 (8)	C13—C8—C9	121.1 (8)
N1—C7—H7	118.7	C13—C8—H8	119.4
C6—C7—H7	118.7	C9—C8—H8	119.4
C4—C5—C6	120.4 (7)	C8—C13—C12	118.8 (9)
C4—C5—H5	119.8	C8—C13—C14	124.6 (10)
C6—C5—H5	119.8	C12—C13—C14	116.5 (9)
C2—C3—C4	119.4 (9)	C15—C14—C13	115.7 (11)
C2—C3—H3	120.3	C15—C14—H14A	108.4
C4—C3—H3	120.3	C13—C14—H14A	108.4
C11—C12—C13	122.1 (8)	C15—C14—H14B	108.4
C11—C12—H12	119.0	C13—C14—H14B	108.4
C13—C12—H12	119.0	H14A—C14—H14B	107.4
O1—C1—C2	118.2 (8)	C3—C2—C1	120.8 (8)
O1—C1—C6	121.6 (7)	C3—C2—H2	119.6
C2—C1—C6	120.2 (8)	C1—C2—H2	119.6
C3—C4—C5	121.5 (8)	C9—C10—C11	118.9 (7)
C3—C4—Br1	120.0 (7)	C9—C10—N1	118.0 (7)
C5—C4—Br1	118.4 (6)	C11—C10—N1	123.0 (7)
C12—C11—C10	118.8 (7)	C14—C15—H15A	109.5
C12—C11—H11	120.6	C14—C15—H15B	109.5
C10—C11—H11	120.6	H15A—C15—H15B	109.5
C5—C6—C1	117.8 (7)	C14—C15—H15C	109.5

C5—C6—C7	121.0 (7)	H15A—C15—H15C	109.5
C1—C6—C7	121.1 (7)	H15B—C15—H15C	109.5
C10—C9—C8	120.1 (8)	C7—N1—C10	121.5 (7)
C10—C9—H9	119.9	C1—O1—H1	109.5
C8—C9—H9	119.9		

C2—C3—C4—C5	1.1 (12)	C9—C8—C13—C14	−178.3 (9)
C2—C3—C4—Br1	177.4 (6)	C11—C12—C13—C8	−1.0 (15)
C6—C5—C4—C3	−0.1 (12)	C11—C12—C13—C14	−179.5 (9)
C6—C5—C4—Br1	−176.5 (6)	C8—C13—C14—C15	−7.7 (18)
C13—C12—C11—C10	−1.2 (13)	C12—C13—C14—C15	170.7 (12)
C4—C5—C6—C1	−1.3 (10)	C4—C3—C2—C1	−0.5 (13)
C4—C5—C6—C7	174.8 (8)	O1—C1—C2—C3	179.3 (8)
O1—C1—C6—C5	−178.5 (7)	C6—C1—C2—C3	−0.9 (13)
C2—C1—C6—C5	1.8 (11)	C8—C9—C10—C11	1.3 (12)
O1—C1—C6—C7	5.4 (11)	C8—C9—C10—N1	177.2 (8)
C2—C1—C6—C7	−174.3 (8)	C12—C11—C10—C9	1.0 (11)
N1—C7—C6—C5	179.7 (8)	C12—C11—C10—N1	−174.7 (7)
N1—C7—C6—C1	−4.3 (12)	C6—C7—N1—C10	170.0 (7)
C10—C9—C8—C13	−3.6 (14)	C9—C10—N1—C7	149.2 (8)
C9—C8—C13—C12	3.4 (15)	C11—C10—N1—C7	−35.1 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.89	2.609 (10)	146