Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Bromo-2-{(*E*)-[(3,4-dimethylphenyl)-imino]methyl}phenol

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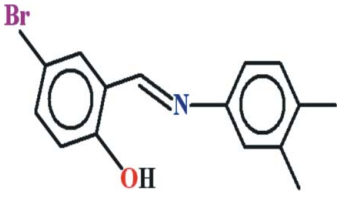
Received 13 August 2012; accepted 13 August 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.073; data-to-parameter ratio = 15.3.

In the title compound, $C_{15}H_{14}BrNO$, the dihedral angle between the aromatic rings is 4.10 (11)° and the molecule is close to planar (r.m.s. deviation for the non-H atoms = 0.053 Å). An intramolecular O—H···N hydrogen bond closes an S(6) ring. In the crystal, very weak C—H···π interactions are observed.

Related literature

For related structures, see: Unver *et al.* (2010). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{15}H_{14}BrNO$
M_r = 304.18
Monoclinic, $P2_1/n$
a = 12.2633 (10) Å
b = 7.4805 (6) Å
c = 14.5767 (11) Å
β = 101.576 (4)°
V = 1310.00 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.13 mm^{-1}
T = 296 K
0.30 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.454, T_{max} = 0.546
9488 measured reflections
2545 independent reflections
1931 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.073
S = 1.04
2545 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.87	2.601 (2)	147
C7—H7B···$Cg1^{i}$	0.96	2.95	3.668 (3)	133
C12—H12···$Cg1^{ii}$	0.93	2.96	3.612 (2)	128

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6936).

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supporting information

Acta Cryst. (2012). E**68**, o2730 [doi:10.1107/S1600536812035635]

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M. Nawaz Tahir, Abdul Haleem Khan, Muhammad Ilyas Tariq, Ishtiaq Hussain and Muhammad Shafiq

S1. Comment

The title compound, (Fig. 1) has been synthesized as a possible ligand for forming different metal complexes. its sturcture is now described. The crystal structures of 3,4-dimethyl-*N*-(3-nitrobenzylidene)aniline and 3,4-dimethyl-*N*-(4-nitro-benzylidene) aniline (Unver *et al.*, 2010) have been published which are related to the title compound.

The title compound is almost planar with r.m.s. deviation of 0.0487 Å, with maximum deviation of 0.1043 (11) Å for Br atom from the mean square plane. There exist intramolecular H-bonding of O—H···N type with *S*(6) ring motif (Bernstein *et al.*, 1995). There exist weak C—H···π interactions (Table 1) in the crystal.

S2. Experimental

Equimolar quantities of 3,4-dimethylaniline and 5-bromosalicylaldehyde were refluxed in methanol along with few drops of acetic acid as catalyst for 1 h. The solution was kept at room temperature which affoarded yellow prisms of the title compound after two days.

S3. Refinement

The H-atoms were positioned geometrically (C–H = 0.93–0.96 Å, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, O) where x = 1.5 for hydroxy & methyl and x = 1.2 for other H-atoms.

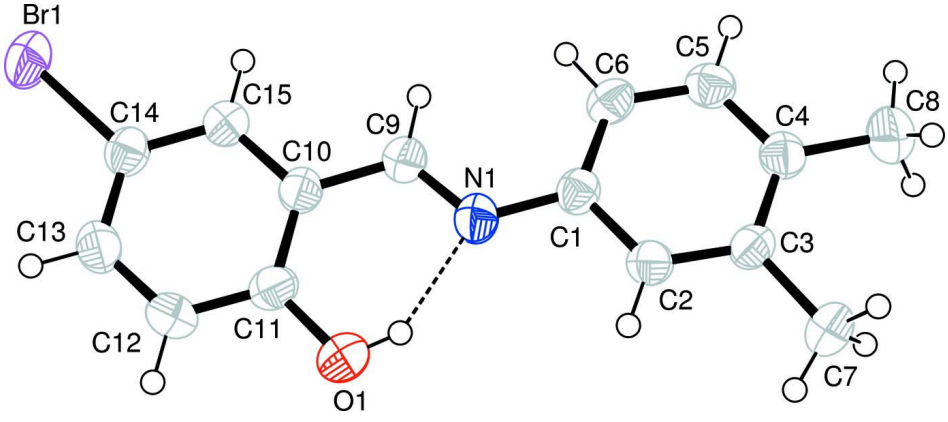

Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level. The dotted line represents the intramolecular hydrogen bond.

4-Bromo-2-{(*E*)-[(3,4-dimethylphenyl)imino]methyl}phenol

Crystal data

$C_{15}H_{14}BrNO$
$M_r = 304.18$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.2633\ (10)$ Å
$b = 7.4805\ (6)$ Å
$c = 14.5767\ (11)$ Å
$\beta = 101.576\ (4)°$
$V = 1310.00\ (18)$ Å^3
$Z = 4$
$F(000) = 616$
$D_x = 1.542$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1931 reflections
$\theta = 2.0–26.0°$
$\mu = 3.13$ mm^{-1}
$T = 296$ K
Prism, yellow
0.30 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.454$, $T_{max} = 0.546$
9488 measured reflections
2545 independent reflections
1931 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.0°$
$h = -10\rightarrow15$
$k = -9\rightarrow8$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.073$
$S = 1.04$
2545 reflections
166 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.1325P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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}
Br1	0.18394 (2)	0.52508 (4)	0.05809 (2)	0.0611 (1)
O1	0.04873 (13)	0.3558 (3)	0.42252 (10)	0.0649 (7)
N1	0.23707 (15)	0.4902 (2)	0.50899 (13)	0.0433 (6)
C1	0.30890 (17)	0.5327 (3)	0.59525 (15)	0.0377 (7)
C2	0.26822 (18)	0.4991 (3)	0.67585 (15)	0.0402 (7)

C3	0.32937 (18)	0.5327 (3)	0.76461 (15)	0.0386 (7)
C4	0.43689 (17)	0.6028 (3)	0.77377 (14)	0.0413 (7)
C5	0.47658 (17)	0.6376 (3)	0.69271 (14)	0.0445 (8)
C6	0.41546 (16)	0.6041 (3)	0.60481 (15)	0.0437 (7)
C7	0.2812 (2)	0.4915 (3)	0.85007 (17)	0.0559 (9)
C8	0.50899 (19)	0.6368 (3)	0.86868 (15)	0.0595 (9)
C9	0.26191 (19)	0.5199 (3)	0.42938 (15)	0.0411 (7)
C10	0.18689 (18)	0.4725 (3)	0.34246 (15)	0.0384 (7)
C11	0.08370 (17)	0.3910 (3)	0.34249 (15)	0.0442 (7)
C12	0.01435 (18)	0.3464 (3)	0.25816 (16)	0.0495 (8)
C13	0.04434 (18)	0.3849 (3)	0.17425 (15)	0.0462 (7)
C14	0.14496 (18)	0.4672 (3)	0.17412 (15)	0.0407 (7)
C15	0.21649 (18)	0.5098 (3)	0.25677 (15)	0.0406 (7)
H1	0.09704	0.38542	0.46739	0.0974*
H2	0.19695	0.45203	0.66987	0.0483*
H5	0.54756	0.68561	0.69831	0.0534*
H6	0.44489	0.62870	0.55214	0.0524*
H7A	0.32881	0.40851	0.88946	0.0838*
H7B	0.20851	0.44010	0.83078	0.0838*
H7C	0.27580	0.59987	0.88418	0.0838*
H8A	0.47412	0.72447	0.90136	0.0893*
H8B	0.58039	0.68003	0.86120	0.0893*
H8C	0.51838	0.52756	0.90395	0.0893*
H9	0.32978	0.57328	0.42700	0.0493*
H12	−0.05316	0.28997	0.25835	0.0594*
H13	−0.00291	0.35554	0.11803	0.0554*
H15	0.28458	0.56350	0.25552	0.0487*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0679 (2)	0.0809 (2)	0.0349 (2)	−0.0060 (1)	0.0114 (1)	0.0038 (1)
O1	0.0642 (11)	0.0893 (14)	0.0442 (9)	−0.0253 (10)	0.0179 (8)	0.0017 (9)
N1	0.0464 (10)	0.0475 (11)	0.0355 (10)	−0.0011 (8)	0.0073 (8)	−0.0028 (8)
C1	0.0431 (12)	0.0358 (11)	0.0349 (11)	0.0024 (9)	0.0094 (9)	−0.0005 (9)
C2	0.0409 (12)	0.0401 (13)	0.0407 (12)	−0.0035 (9)	0.0105 (10)	−0.0015 (9)
C3	0.0461 (12)	0.0359 (12)	0.0359 (11)	0.0004 (10)	0.0135 (9)	0.0012 (9)
C4	0.0468 (12)	0.0348 (12)	0.0411 (12)	0.0005 (10)	0.0059 (10)	0.0003 (10)
C5	0.0379 (12)	0.0455 (14)	0.0498 (14)	−0.0034 (10)	0.0080 (10)	0.0022 (10)
C6	0.0436 (13)	0.0494 (13)	0.0413 (12)	−0.0001 (10)	0.0160 (10)	0.0036 (10)
C7	0.0664 (16)	0.0653 (17)	0.0388 (13)	−0.0078 (12)	0.0173 (12)	0.0006 (10)
C8	0.0621 (15)	0.0662 (18)	0.0460 (14)	−0.0063 (13)	0.0005 (12)	−0.0015 (12)
C9	0.0439 (12)	0.0426 (13)	0.0371 (12)	−0.0022 (10)	0.0091 (9)	−0.0008 (9)
C10	0.0435 (12)	0.0362 (12)	0.0352 (12)	0.0007 (9)	0.0074 (9)	0.0001 (9)
C11	0.0487 (13)	0.0442 (13)	0.0420 (12)	−0.0054 (11)	0.0146 (10)	0.0032 (10)
C12	0.0444 (13)	0.0498 (15)	0.0529 (14)	−0.0121 (10)	0.0063 (11)	−0.0003 (11)
C13	0.0487 (13)	0.0445 (13)	0.0414 (12)	−0.0010 (11)	−0.0006 (10)	−0.0014 (10)
C14	0.0460 (13)	0.0399 (12)	0.0365 (12)	0.0045 (10)	0.0089 (10)	−0.0001 (9)

C15	0.0414 (12)	0.0416 (13)	0.0391 (12)	−0.0006 (9)	0.0091 (10)	0.0009 (9)

Geometric parameters (Å, º)

Br1—C14	1.898 (2)	C12—C13	1.377 (3)
O1—C11	1.347 (3)	C13—C14	1.379 (3)
O1—H1	0.8200	C14—C15	1.378 (3)
N1—C1	1.419 (3)	C2—H2	0.9300
N1—C9	1.277 (3)	C5—H5	0.9300
C1—C6	1.393 (3)	C6—H6	0.9300
C1—C2	1.388 (3)	C7—H7A	0.9600
C2—C3	1.382 (3)	C7—H7B	0.9600
C3—C4	1.400 (3)	C7—H7C	0.9600
C3—C7	1.514 (3)	C8—H8A	0.9600
C4—C8	1.507 (3)	C8—H8B	0.9600
C4—C5	1.390 (3)	C8—H8C	0.9600
C5—C6	1.372 (3)	C9—H9	0.9300
C9—C10	1.452 (3)	C12—H12	0.9300
C10—C15	1.397 (3)	C13—H13	0.9300
C10—C11	1.405 (3)	C15—H15	0.9300
C11—C12	1.388 (3)		
C11—O1—H1	109.00	C1—C2—H2	119.00
C1—N1—C9	123.19 (19)	C3—C2—H2	119.00
N1—C1—C6	125.30 (19)	C4—C5—H5	119.00
C2—C1—C6	118.3 (2)	C6—C5—H5	119.00
N1—C1—C2	116.41 (19)	C1—C6—H6	120.00
C1—C2—C3	122.7 (2)	C5—C6—H6	120.00
C2—C3—C7	120.4 (2)	C3—C7—H7A	109.00
C4—C3—C7	120.89 (19)	C3—C7—H7B	109.00
C2—C3—C4	118.8 (2)	C3—C7—H7C	109.00
C3—C4—C8	121.25 (19)	H7A—C7—H7B	110.00
C5—C4—C8	120.53 (19)	H7A—C7—H7C	109.00
C3—C4—C5	118.22 (19)	H7B—C7—H7C	109.00
C4—C5—C6	122.8 (2)	C4—C8—H8A	109.00
C1—C6—C5	119.3 (2)	C4—C8—H8B	109.00
N1—C9—C10	121.7 (2)	C4—C8—H8C	109.00
C9—C10—C11	121.2 (2)	H8A—C8—H8B	109.00
C9—C10—C15	119.9 (2)	H8A—C8—H8C	109.00
C11—C10—C15	118.9 (2)	H8B—C8—H8C	109.00
O1—C11—C10	121.90 (19)	N1—C9—H9	119.00
O1—C11—C12	118.36 (19)	C10—C9—H9	119.00
C10—C11—C12	119.7 (2)	C11—C12—H12	120.00
C11—C12—C13	120.8 (2)	C13—C12—H12	120.00
C12—C13—C14	119.6 (2)	C12—C13—H13	120.00
Br1—C14—C13	119.24 (16)	C14—C13—H13	120.00
C13—C14—C15	121.0 (2)	C10—C15—H15	120.00
Br1—C14—C15	119.77 (17)	C14—C15—H15	120.00

C10—C15—C14	120.1 (2)		
C9—N1—C1—C2	177.4 (2)	N1—C9—C10—C11	−0.3 (3)
C9—N1—C1—C6	−2.7 (3)	N1—C9—C10—C15	179.0 (2)
C1—N1—C9—C10	179.2 (2)	C9—C10—C11—O1	1.1 (3)
N1—C1—C2—C3	179.5 (2)	C9—C10—C11—C12	−179.6 (2)
C6—C1—C2—C3	−0.4 (3)	C15—C10—C11—O1	−178.2 (2)
N1—C1—C6—C5	−179.5 (2)	C15—C10—C11—C12	1.1 (3)
C2—C1—C6—C5	0.4 (3)	C9—C10—C15—C14	−179.2 (2)
C1—C2—C3—C4	−0.3 (3)	C11—C10—C15—C14	0.2 (3)
C1—C2—C3—C7	−179.3 (2)	O1—C11—C12—C13	177.8 (2)
C2—C3—C4—C5	0.8 (3)	C10—C11—C12—C13	−1.5 (3)
C2—C3—C4—C8	−178.0 (2)	C11—C12—C13—C14	0.6 (3)
C7—C3—C4—C5	179.9 (2)	C12—C13—C14—Br1	−178.45 (17)
C7—C3—C4—C8	1.0 (3)	C12—C13—C14—C15	0.7 (3)
C3—C4—C5—C6	−0.8 (3)	Br1—C14—C15—C10	178.07 (17)
C8—C4—C5—C6	178.1 (2)	C13—C14—C15—C10	−1.1 (3)
C4—C5—C6—C1	0.2 (4)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.87	2.601 (2)	147
C7—H7*B*···*Cg*1^{i}	0.96	2.95	3.668 (3)	133
C12—H12···*Cg*1^{ii}	0.93	2.96	3.612 (2)	128

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+3/2; (ii) *x*−1/2, −*y*+1/2, *z*−1/2.