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(*E*)-2-[(3-Bromophenylimino)methyl]-6-methylphenol

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.081
Data-to-parameter ratio = 18.9

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

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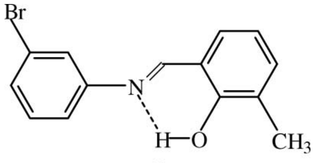
The title compound, $C_{14}H_{12}BrNO$, crystallizes in a phenol–imine tautomeric form. The structure is stabilized by O—H···N intramolecular hydrogen bonds, C—H···π and π–π intermolecular interactions. The molecule is planar and intramolecular O—H···N hydrogen bonding generates an S(6) ring motif.

Comment

Schiff bases have biological activities and they are widely used as ligands in metal comlexes (Calligaris & Randaccio 1987). *o*-Hydroxy Schiff bases derived from the reaction of *o*-hydroxyaldehydes with aniline have been extensively examined (Stewart & Lingafelter, 1959; Calligaris *et al.*, 1972). There are two types of intramolecular hydrogen bonds in Schiff bases, *viz*. keto–amine (N—H···O) and phenol–imine (N···H—O) tautomeric forms. In the title compound, (I), the phenol–imine tautomer is favoured over the keto–amine tautomer.



(I)

The molecular structure is shown in Fig. 1. The molecule is planar, the dihedral angle formed by the mean planes of the C1–C6 and C8–C13 aromatic rings being 0.44 (16)°. The C2—O1 and C7═N1 bond lengths are 1.348 (3) and 1.273 (3) Å, respectively, in agreement with the corresponding distances in

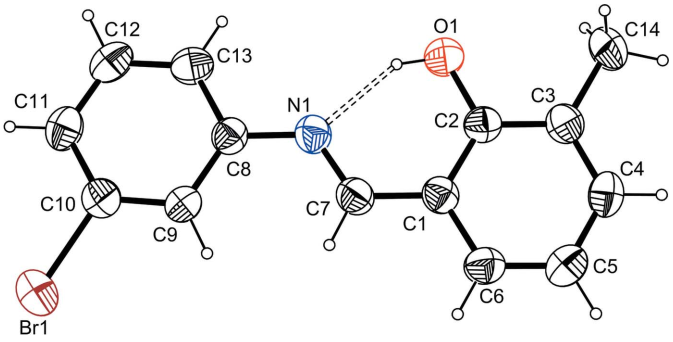


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms are represented as small spheres of arbitrary radius. The hydrogen bond is shown as a double-dashed line.

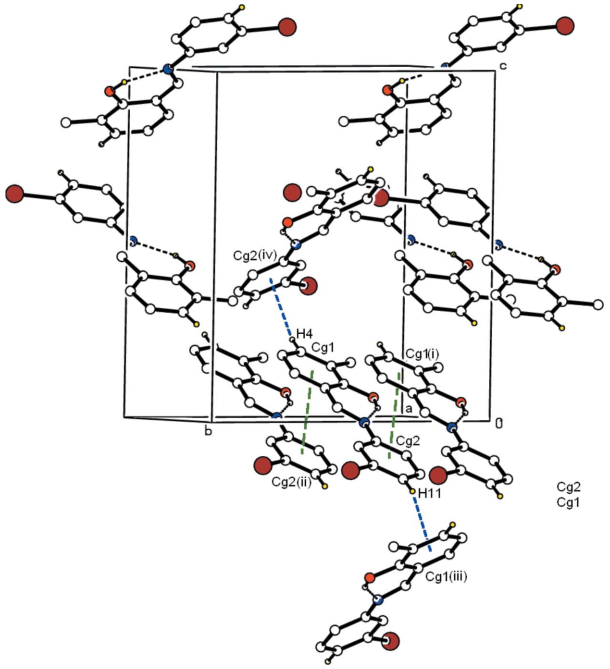


Figure 2
A partial packing view of the title compound, showing the C—H···π interactions and π–π stacking (dashed lines). H atoms not participating in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) $\frac{1}{2} - x, 1 - y, \frac{1}{2} + z$; (ii) $-\frac{1}{2} - x, 1 - y, z - \frac{1}{2}$; (iii) $1 + x, y, z$; (iv) $-1 + x, y, z$.]

2-[2-(hydroxymethyl)phenyliminomethyl]phenol [1.354 (2) and 1.275 (2) Å; Ersanlı *et al.*, 2004]. There is a strong intramolecular O—H···N hydrogen bond in (I) (Table 1), which is a common feature of phenol–imine systems. Fig. 1 also shows the strong intramolecular hydrogen bond (O1—H1···N1), which gives rise to a six-membered *S*6 pseudo-ring (Bernstein *et al.*, 1995). The O1···N1 distance of 2.614 (3) Å is comparable to those observed for analogous hydrogen bonds in 2-[2-(hydroxymethyl)phenyliminomethyl]phenol [2.614 (2) Å; Ersanlı *et al.*, 2004].

C—H···π intermolecular and π–π stacking interactions play an appreciable role in determining the conformation of organic compounds (Umezawa *et al.*, 1999). C—H···π interactions are reported in Table 1. In addition, there is a weak offset π–π stacking interaction between the $Cg1\cdots Cg2^{iii}$ rings, with the centroid-to-centroid distance of 3.655 (2) Å [*Cg*1 is the centroid of the C1–C6 ring and *Cg*2 is centroid of the C8–C13 ring; symmetry code: (iii) 1 + *x*, *y*, *z*]. These interactions pack the structure along the [010] direction.

Experimental

The compound (*E*)-2-[(3-bromophenylimino)methyl]-6-methylphenol was prepared by refluxing a mixture of a solution containing 3-methylsalicylaldehyde (0.1 ml 0.82 mmol) in 20 ml ethanol and a solution containing 3-bromoaniline (0.14 g 0.82 mmol) in 20 ml ethanol. The reaction mixture was stirred for 2 h under reflux. Crystals of (*E*)-2-[(3-bromophenylimino)methyl]-6-methylphenol suitable for X-ray analysis were obtained from ethyl alcohol by slow evaporation (yield 59%; m.p. 352–354 K).

Crystal data

$C_{14}H_{12}BrNO$
$M_r = 290.16$
Orthorhombic, $P2_12_12_1$
$a = 6.2637$ (5) Å
$b = 13.8902$ (11) Å
$c = 14.3678$ (15) Å
$V = 1250.06$ (19) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 3.28$ mm^{-1}
$T = 296$ K
0.57 × 0.46 × 0.33 mm

Data collection

Stoe IPDS-2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe, 2002)
$T_{min} = 0.204$, $T_{max} = 0.451$
8829 measured reflections
2971 independent reflections
2326 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.081$
$S = 1.04$
2971 reflections
157 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Absolute structure: Flack (1983), 1228 Friedel pairs
Flack parameter: 0.02 (1)

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O1—H1···N1	0.82	1.88	2.614 (3)	148
$C4—H4\cdots Cg2^{i}$	0.93	2.75	3.529 (3)	142
$C11—H11\cdots Cg1^{ii}$	0.93	2.72	3.526 (3)	146

Symmetry codes: (i) $-x + \frac{1}{2}, -y + 1, z + \frac{1}{2}$; (ii) $-x - \frac{1}{2}, -y + 1, z - \frac{1}{2}$. *Cg*1 is the centroid of the C1–C6 ring and *Cg*2 is centroid of the C8–C13 ring;.

H atoms were positioned geometrically (O—H = 0.82, C—H = 0.93 for aromatic, 0.98 for C*sp*^{2} and 0.96 Å for methyl) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}$(O, methyl C).

Data collection: *X-AREA* (Stoe, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe, 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) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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