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N-(4-Bromobenzylidene)-2,4-dimethylaniline

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.044
wR factor = 0.137
Data-to-parameter ratio = 17.2

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

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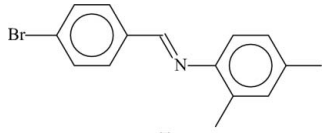
The molecule of the title compound, $C_{15}H_{14}BrN$, is twisted along the C═N bond, the dihedral angle between the aromatic rings being 56.5 (1)°.

Comment

Two previous studies have detailed the crystal structures of the Schiff bases that are synthesized by condensing 4-bromobenzaldehyde and a substituted aniline (Jiao *et al.*, 2006; Sun *et al.*, 2006). The compound that is derived by condensing the aldehyde with 2,4-dimethylaniline exists as a non-planar molecule that is twisted about the imino C═N bond, the dihedral angle between the two aromatic rings being 56.5 (1)°.



(I)

Experimental

4-Bromobenzaldehyde (1.85 g, 10 mmol) and 2,4-dimethylaniline (1.26 ml, 10 mmol) were dissolved in ethanol (30 ml) along with 1 ml formic acid. The solution was refluxed for 6 h. The removal of the solvent and recrystallization from a 1:1 ethanol–dichloromethane mixture (30 ml) gave the compound in about 75% yield. Crystals were grown from ethanol as solvent. Elemental analysis calculated for $C_{15}H_{14}BrN$: C 65.52, H 4.90, N 4.86%; found: C 62.29, H 4.81, N 4.90%.

Crystal data

$C_{15}H_{14}BrN$
M_r = 288.18
Monoclinic, *Cc*
a = 7.554 (1) Å
b = 15.323 (1) Å
c = 11.714 (1) Å
β = 97.134 (1)°
V = 1345.5 (2) Å^3
Z = 4
D_x = 1.423 Mg m^{-3}
Mo *Kα* radiation
μ = 3.03 mm^{-1}
T = 293 (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

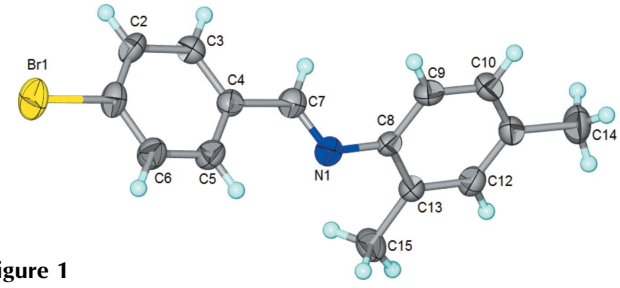


Figure 1
The molecular structure of (I), with displacement ellipsoids plotted at the 50% probablity level and H atoms as spheres of arbitrary radii.

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.411, T_{max} = 0.582
(expected range = 0.385–0.545)

5715 measured reflections
2708 independent reflections
2328 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.137
S = 1.06
2708 reflections
157 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2 + 1.3037P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 1169 Friedel pairs
Flack parameter: 0.03 (2)

H atoms were placed in calculated positions [C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C)], and were included in the refinement in the riding-model approximation. The methyl groups were rotated to fit the electron density.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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