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5-Bromosalicylaldehyde benzoylhydrazone

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.031
wR factor = 0.067
Data-to-parameter ratio = 12.7

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

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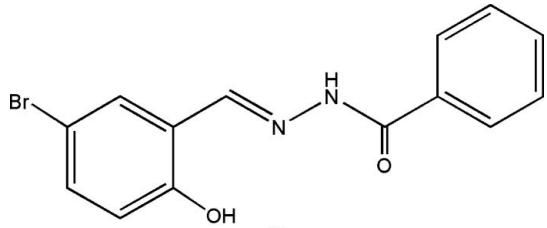
The title compound, $C_{14}H_{11}BrN_2O_2$, was synthesized by the reaction of 5-bromosalicylaldehyde with benzoylhydrazine. Intermolecular N—H···O hydrogen bonds link the molecules into chains running along the *a* axis. The crystal packing is further stabilized by van der Waals forces.

Comment

The coordination chemistry of substituted hydrazones has received much impetus by the remarkable anticancer, amoebicidal, antibacterial, antimicrobial and antileukaemic activities exhibited by these compounds which can be related to their metal-complexing abilities (Wester & Palenik, 1973). The chemical and pharmacological properties of aroylhydrazones have been extensively investigated owing to their potential applications as antineoplastic, antiviral, anti-inflammatory (Bino *et al.*, 1987; Constable *et al.*, 1987) and antitumour agents (Booth *et al.*, 1971). We report here the crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), all bond lengths and angles show normal values (Allen *et al.*, 1987). The N1—C1 and N1—N2 bond lengths are 1.275 (4) and 1.362 (5) Å, respectively. The hydroxy group is involved in an intramolecular O—H···N hydrogen bond (Table 1). The phenyl ring and mean plane of O1/N1/N2/C1–C7 make a dihedral angle of 41.94 (13)°.

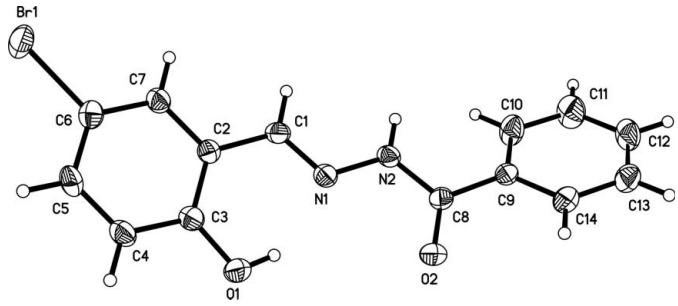


Figure 1
The molecular structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme.

Intermolecular N—H···O hydrogen bonds link the molecules into chains running along the *a* axis. The crystal packing (Fig. 2) is further stabilized by van der Waals forces

Experimental

The title compound was synthesized by the reaction of 5-bromosalicylaldehyde (5 mmol) with benzoylhydrazine (5 mmol). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{14}H_{11}BrN_2O_2$
M_r = 319.16
Orthorhombic, $Pna2_1$
a = 9.534 (3) Å
b = 9.970 (2) Å
c = 13.783 (3) Å
V = 1310.2 (6) Å^3
Z = 4
D_x = 1.618 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.14 mm^{-1}
T = 298 (2) K
Block, colourless
0.42 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.353, T_{max} = 0.651
6496 measured reflections
2191 independent reflections
1747 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.067
S = 1.00
2191 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.028P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}
Absolute structure: Flack (1983), 983 Friedel pairs
Flack parameter: −0.003 (12)

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	2.590 (4)	143
N2—H2···O2^{i}	0.86	2.11	2.924 (4)	157

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

H atoms were placed in geometrically idealized positions (N—H = 0.86 Å, O—H = 0.82 Å and C—H = 0.93 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(O).

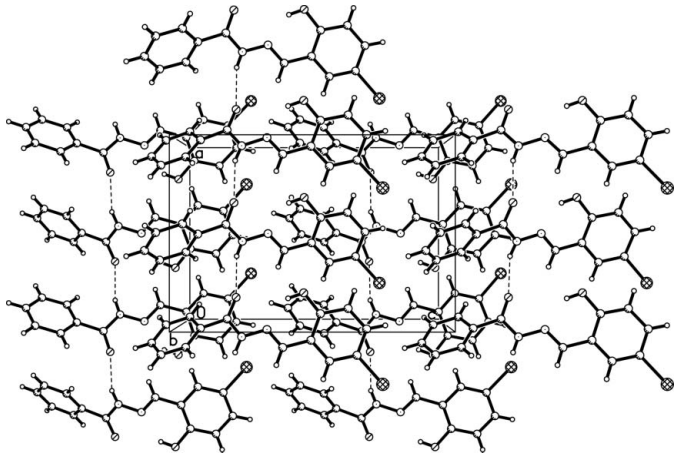


Figure 2
A packing diagram of (I), viewed down the *b* axis. Dashed lines denote the N—H···O hydrogen bonds.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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