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# 2-Hydroxy-2′-(4-isopropylbenzylidene)-benzohydrazide

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**Key indicators**

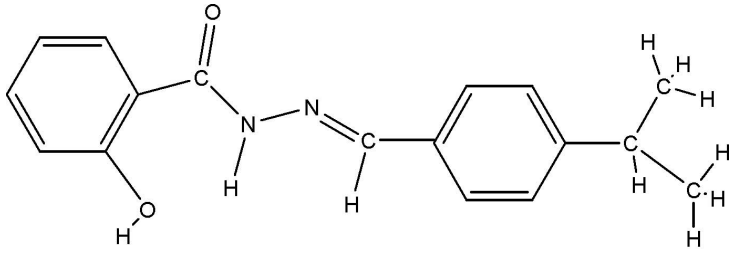
Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.005 Å
*R* factor = 0.076
*wR* factor = 0.228
Data-to-parameter ratio = 15.2

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

The title compound, $C_{17}H_{18}N_2O_2$, was synthesized by the reaction of 2-hydroxybenzoylhydrazine with 4-isopropylbenzaldehyde in ethanol. The molecule is non-planar and the dihedral angle between the two aromatic rings is 21.9 (2)°. The crystal structure involves intermolecular O—H···O and intramolecular N—H···O hydrogen bonds.

## Comment

Some benzoylhydrazone compounds possess bacteriostatic activity. This type of compound has wide application in tuberculosis treatment and also exhibits fungicidal activity (Edwards *et al.*, 1975). Some hydrazonecarbonyl compounds also show bioactivity (Zhi *et al.*, 2003; Yang & Pan, 2004). In order to explore more effective antibacterial medicines, we have synthesized the title compound, (I).



(I)

The title molecule (Fig. 1) is non planar; the dihedral angle between the two aromatic rings is 22.0 (2)°. As a result of conjugation, the C═O distance [1.227 (3) Å] is longer than the normal value of 1.21 Å (Dean, 1998), and the C1—N1 bond distance [1.341 (4) Å] is longer than the C═N double-bond distance (1.32 Å; Dean, 1998) and shorter than the C—N single-bond distance (1.475 Å; Dean, 1998).

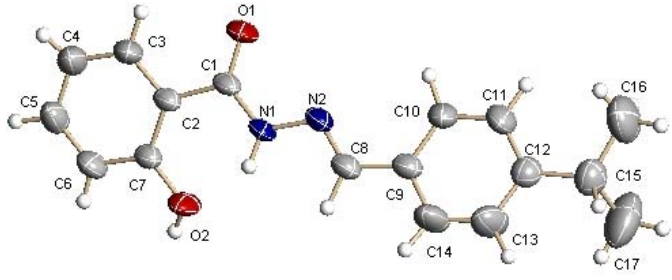



**Figure 1**
Structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 30% probability level.

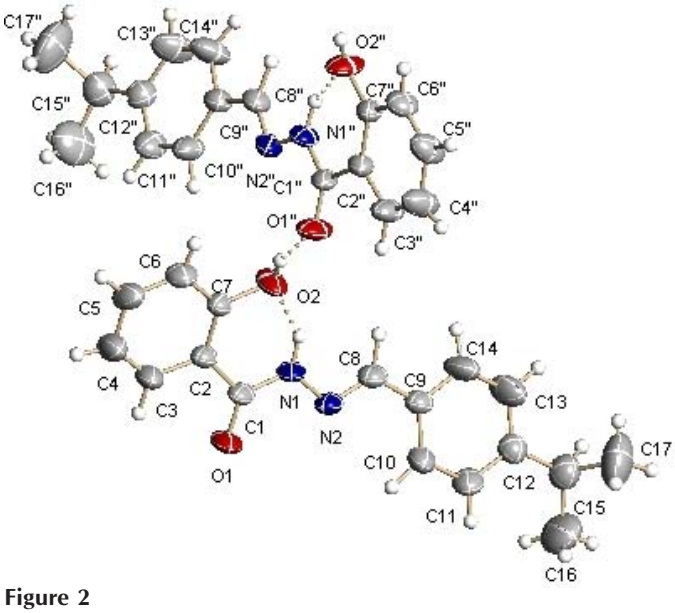



**Figure 2**
Packing of (I), showing the intermolecular and intramolecular hydrogen bonds as dotted lines.

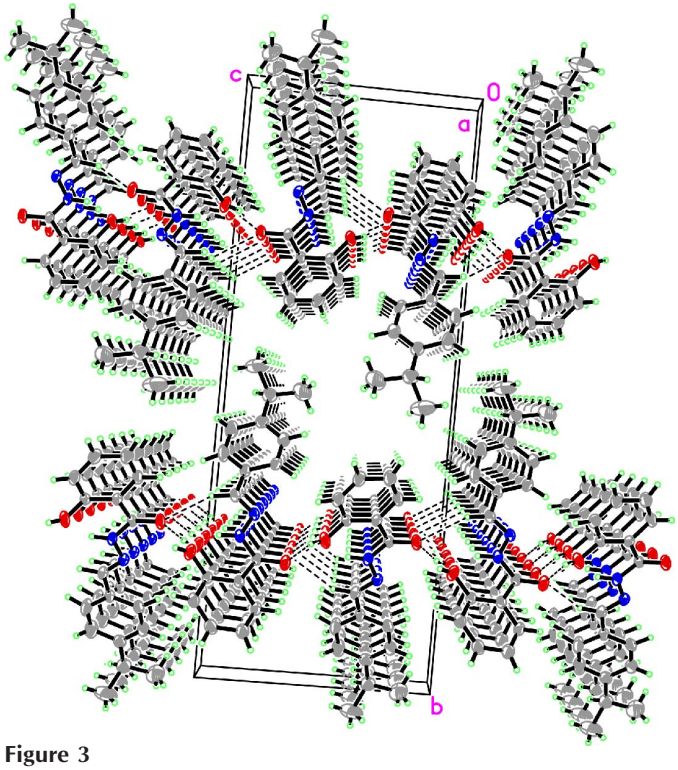



**Figure 3**
Packing of (I), viewed down the *a* axis, showing hydrogen-bonded chains. Hydrogen bonding is shown as dashed lines.

An intramolecular N1—H1···O2 hydrogen bond, which forms a six-membered ring, is observed between the NH group and the hydroxy O atom (Fig. 2). In addition, an intermolecular O2—H2···O1$^{i}$ [symmetry code: (i) $\frac{1}{2}+x, \frac{1}{2}-y, z-\frac{1}{2}$] hydrogen bond is observed, linking the hydroxy H atom with the keto group of an adjacent molecule. The symmetry-related molecules are linked along the *c*-axis direction *via* O—H···O hydrogen bonds to form a chain (Fig. 3).

## Experimental

2-Hydroxybenzoylhydrazine (0.02 mol, 3.04 g) was dissolved in anhydrous ethanol (50 ml), and 4-isopropylbenzaldehyde (0.02 mol, 2.96 g) was added. The mixture was refluxed for 6 h and the resulting precipitate was collected by filtration and washed with ethanol. The product was recrystallized from ethanol and dried under reduced pressure to give the title compound. The compound (2.0 mmol, 0.56 g) was dissolved in dimethylformamide (30 ml) and kept at room temperature for 42 d to obtain colourless single crystals, which were collected and washed with distilled water (m.p. 519–520 K). IR (KBr, cm$^{-1}$): $\nu_{max}$ 2951, 2925, 1629, 1612, 1558, 1457, 1380, 1311, 1238, 1155, 747. $^1$H NMR (200 MHz, DMSO): $\delta$ 11.92 (2H), 8.44 (1H), 7.95 (1H), 7.83 (2H), 7.40 (3H), 6.95 (2H), 2.95 (1H), 1.22 (6H).

### *Crystal data*

$C_{17}H_{18}N_2O_2$
$M_r$ = 282.33
Monoclinic, $P2_1/n$
$a$ = 4.9264 (19) Å
$b$ = 28.000 (11) Å
$c$ = 11.098 (4) Å
$\beta$ = 97.957 (7)°
$V$ = 1516.1 (10) Å$^3$
$Z$ = 4
$D_x$ = 1.237 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1484 reflections
$\theta$ = 4.7–45.4°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 (2) K
Block, colourless
0.35 × 0.33 × 0.08 mm

### *Data collection*

Bruker APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.972, $T_{max}$ = 0.994
8199 measured reflections
3116 independent reflections
1720 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.107
$\theta_{max}$ = 26.5°
$h = -6 \rightarrow 6$
$k = -34 \rightarrow 35$
$l = -13 \rightarrow 7$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.228
$S$ = 1.03
3116 reflections
205 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1071P)^2$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

**Table 1**
Selected interatomic distances (Å).

| | | | |
|---|---|---|---|
| O1—C1 | 1.227 (3) | N1—C1 | 1.341 (4) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2 | 0.85 (3) | 1.96 (3) | 2.630 (3) | 135 (3) |
| O2—H2···O1$^{i}$ | 0.86 (2) | 1.82 (2) | 2.653 (3) | 161 (4) |

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

Atoms H1, H2 and H15 were located in a difference map and their parameters were refined. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 or 0.96 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C). For the refined H atoms, N—H = 0.85 (3) Å, O—H = 0.862 (19) Å and C—H = 1.02 (4) Å.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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## References

Bruker (2002). *SMART* (Version 5.62), *SAINT* (Version 6.02), *SADABS* (Version 2.03) and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Dean, J. A. (1998). Editor. *Lang's Handbook of Chemistry*, Vol. 4, pp. 39–41. New York: McGraw-Hill.

Edwards, E. I., Epton, R. & Marr, G. (1975). *J. Organomet. Chem.* **85**, C23–C25.

Yang, J. G. & Pan, F. Y. (2004). *Acta Cryst.* E**60**, o2009–o2010.

Zhi, J. F., Bin, Z., Su, H. W. & Zheng, M. L. (2003). *Chin. J. Appl. Chem.* **20**, 365–367.