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3-Hydroxysalicylaldehyde 2-furoylhydrazone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.127
Data-to-parameter ratio = 12.1

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

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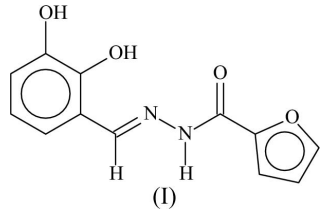
The molecule of the title compound, $C_{12}H_{10}N_2O_4$, is planar and two molecules are stacked over one another at a distance of 3.6 Å. The molecules are linked by hydrogen bonds into a three-dimensional network.

Comment

Among the salicylaldehyde–benzoylhydrazone class of Schiff bases, some require intermolecular hydrogen bonds to stabilize a planar conformation (Huo *et al.*, 2004). A previous study by our group described the non-planar structure of 3-hydroxysalicylaldehyde benzoylhydrazone (Ali *et al.*, 2005).



(I)

In the title compound, (I) (Fig. 1), the 3-hydroxy substituent forms an intermolecular hydrogen bond to the carbonyl O atom of an adjacent molecule. In addition, this unit is also an acceptor of the amino H atom. The planar molecules are stacked over one another (Fig. 2), and the molecules are linked by hydrogen bonds (Table 2) into a three-dimensional network. The O atom of the furyl ring does not participate in any hydrogen bonding. Salicylaldehyde 2-furoylhydrazone has been reported but its structure has not yet been determined (Garg *et al.*, 2000).

Experimental

3-Hydroxysalicyldehyde (0.28 g, 2 mmol) and 2-furoylhydrazide (0.25 g, 2 mmol) were heated in ethanol (40 ml) for 2 h. Compound (I) separated from the solution as yellow plates.

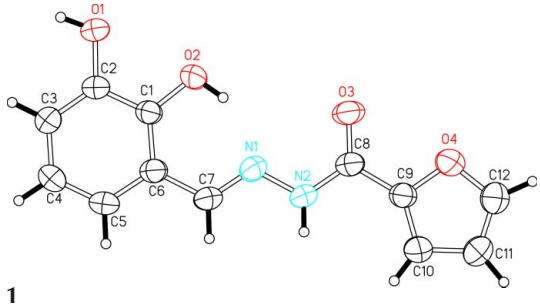


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

Crystal data

$C_{12}H_{10}N_2O_4$
M_r = 246.22
Monoclinic, $P2_1/n$
a = 11.2143 (8) Å
b = 9.3730 (7) Å
c = 11.4149 (9) Å
β = 109.120 (1)°
V = 1133.7 (2) Å^3
Z = 4
D_x = 1.443 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2381 reflections
θ = 2.2–27.0°
μ = 0.11 mm^{-1}
T = 295 (2) K
Plate, yellow
0.42 × 0.32 × 0.14 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: none
6280 measured reflections
2461 independent reflections
1703 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.0°
$h = -13 \rightarrow 14$
$k = -11 \rightarrow 11$
$l = -9 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.127
S = 1.03
2461 reflections
203 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 0.2675P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.368 (2)	O4—C12	1.348 (3)
O2—C1	1.359 (2)	N1—N2	1.371 (2)
O3—C8	1.233 (2)	N1—C7	1.280 (2)
O4—C9	1.358 (2)	N2—C8	1.344 (2)
C9—O4—C12	106.3 (2)	O3—C8—C9	121.8 (2)
N2—N1—C7	118.3 (1)	N2—C8—C9	115.3 (1)
N1—N2—C8	117.5 (1)	O4—C9—C8	114.5 (1)
N1—C7—C6	119.7 (2)	O4—C9—C10	109.5 (2)
O3—C8—N2	122.8 (2)		
C1—C6—C7—N1	1.3 (3)	N1—N2—C8—O3	−1.3 (2)
C7—N1—N2—C8	178.6 (2)	N1—N2—C8—C9	177.8 (1)
C6—C7—N1—N2	179.8 (2)	O3—C8—C9—O4	5.3 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*o*···O3^{i}	0.86 (1)	1.82 (1)	2.662 (2)	169 (2)
O2—H2*o*···N1	0.86 (1)	1.85 (2)	2.611 (2)	147 (2)
N2—H2*n*···O1^{ii}	0.85 (1)	2.18 (2)	2.890 (2)	141 (2)

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

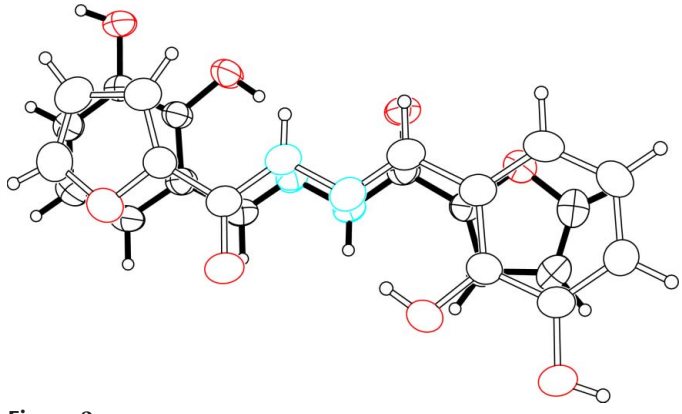


Figure 2
A plot illustrating the π–π stacking of molecules of (I). The C, N and O atoms shown without principal axes are related to those shown with principal axes by $(1-x, 2-y, 1-z)$.

The carbon-bound H atoms were refined with a distance restraint of 0.95 (1) Å, and the nitrogen- and oxygen-bound H atoms with a distance restraint of 0.85 (1) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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