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2′-(1,3-Benzodioxol-5-ylmethylene)furan-2-carbohydrazide

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Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.160
Data-to-parameter ratio = 15.4

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

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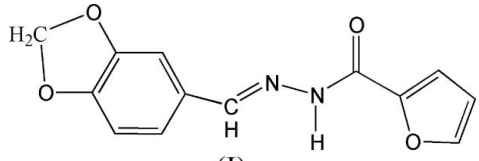
In the title molecule, $C_{13}H_{10}N_2O_4$, the dihedral angle between the benzodioxole ring system and the furan ring is 18.7 (1)°. Intermolecular N—H···O and C—H···O hydrogen bonds link the molecules into a three-dimensional framework.

Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of an investigation of the coordination properties of Schiff bases functioning as ligands, we report the synthesis and structure of the title compound, (I).



(I)

In the molecular structure of (I) (Fig. 1), the expected geometric parameters are observed. The benzodioxole ring system (C7–C13/O3/O4) is planar, with an r.m.s. deviation for the fitted atoms of 0.0154 (6) Å, as is the furan ring (C2–C5/O2), with an r.m.s. deviation of 0.0009 (5) Å. The dihedral angle between these two planes is 18.7 (1)°.

Intermolecular N—H···O hydrogen bonds link the molecules into chains running along the *a* axis. These chains are cross-linked *via* C—H···O hydrogen bonds (Table 1) forming a network structure, as illustrated in Fig. 2.

Experimental

An anhydrous ethanol solution (50 ml) of benzo[1,3]dioxole-5-carbaldehyde (1.50 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of furan-2-carboxylic acid hydrazide (1.26 g, 10 mmol), and the mixture was stirred at 350 K for 6 h under N_2, yielding a red solution. The solvent was removed and the residue was recrystallized from anhydrous ethanol. The product was isolated and then dried *in vacuo* to give pure compound (I) in 91% yield. Red single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution.

Crystal data

$C_{13}H_{10}N_2O_4$
M_r = 258.23
Monoclinic, $P2_1/a$
a = 9.8351 (7) Å
b = 11.3996 (8) Å
c = 10.4260 (7) Å
β = 95.079 (3)°
V = 1164.33 (14) Å^3
Z = 4
D_x = 1.473 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 113 (2) K
Prism, red
0.22 × 0.18 × 0.16 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.982
10631 measured reflections
2704 independent reflections
1672 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 27.9°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.160
S = 1.07
2704 reflections
176 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.085P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.93 (2)	2.01 (2)	2.843 (2)	150 (2)
C4—H4···O4^{ii}	0.95	2.51	3.441 (3)	168
C5—H5···O3^{iii}	0.95	2.38	3.143 (3)	137
C6—H6···O1^{i}	0.95	2.57	3.193 (2)	124
C13—H13B···O1^{iv}	0.99	2.35	3.284 (2)	158

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

The N-bound H atom was located in a difference Fourier map and its positional parameters were refined, with U_{iso}(H) = 1.5U_{eq}(N). C-bound H atoms were included in calculated positions, with C—H = 0.95 (aromatic) or 0.99 Å (methylene), and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1996); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

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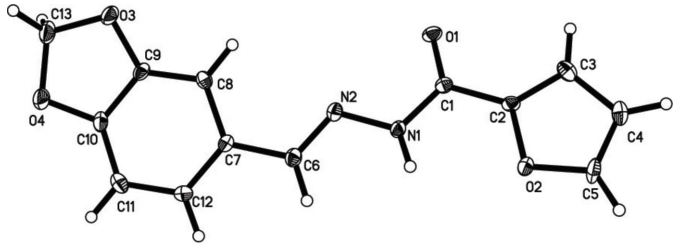

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

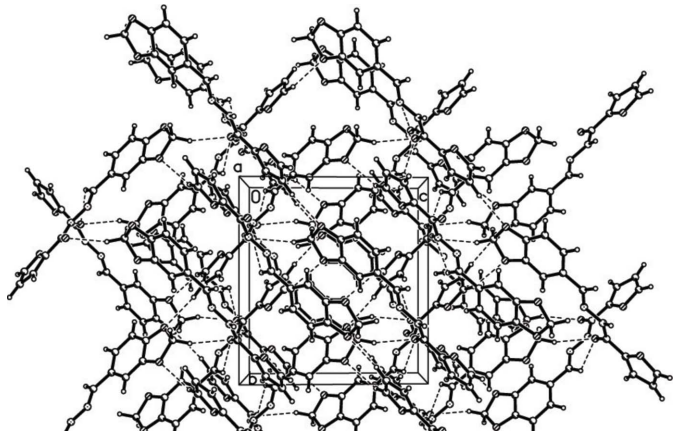

Figure 2
The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are indicated by dashed lines.

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