Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-[1-(2-Furyl)ethenyl]propanohydrazide

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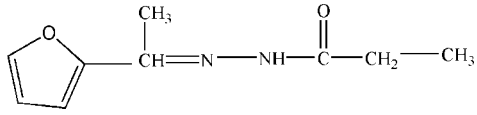
Received 17 June 2007; accepted 19 December 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.149; data-to-parameter ratio = 15.8.

The title compound, $C_9H_{12}N_2O_2$, was prepared by the reaction of acetylfuran and propionylhydrazine. The molecule, excluding H atoms, is approximately planar. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds.

Related literature

For related literature on similar compounds, see: Cimerman *et al.* (1997); Sutherland & Hoy (1968); Tucker *et al.* (1975).



Experimental

Crystal data

$C_9H_{12}N_2O_2$
M_r = 180.21
Triclinic, $P\overline{1}$
a = 4.3314 (13) Å
b = 9.560 (3) Å
c = 11.695 (4) Å
α = 102.338 (6)°
β = 98.665 (5)°
γ = 91.273 (5)°
V = 466.9 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.38 × 0.14 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
2708 measured reflections
1893 independent reflections
1188 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.149
S = 1.01
1893 reflections
120 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	2.08	2.925 (2)	166

Symmetry code: (i) $-x-1, -y, -z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RT2014).

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  doi:10.1107/S1600536807067669

supporting information

Acta Cryst. (2008). E**64**, o508 [doi:10.1107/S1600536807067669]

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S1. Comment

Schiff bases have received considerable attention in the literature, and are attractive from several points of view, such as the possibility of analytical application (Cimerman, *et al.*, 1997). As part of our search for new schiff base compounds, we synthesized the title compound (I). The C7—N2 bond length [1.343 (2) Å] is longer than the typical value for a double bond, but less than for a single bond, due to conjugation effects within the molecule.

Bond lengths and angles in the phenyl ring are normal. The C5—N1 distance of 1.280 (2) Å is similar to the similar distance of 1.287 (2) Å reported in a corresponding compound (Tucker *et al.*, 1975). Similarly, the C7—O2 distance of 1.226 (2) Å is shorter than the similar distance of 1.298 (2) Å reported by Sutherland *et al.*, 1968.

S2. Experimental

A mixture of the acetyl furan (11 g, 0.10 mol), and propionylhydrazine (8.8 g, 0.10 mol) was stirred in refluxing ethanol (30 ml) for 5 h to afford the title compound (17 g, 0.087 mol, yield 87%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

S3. Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93–0.98 Å, and with U_{iso}=1.2–1.5U_{eq}(C).

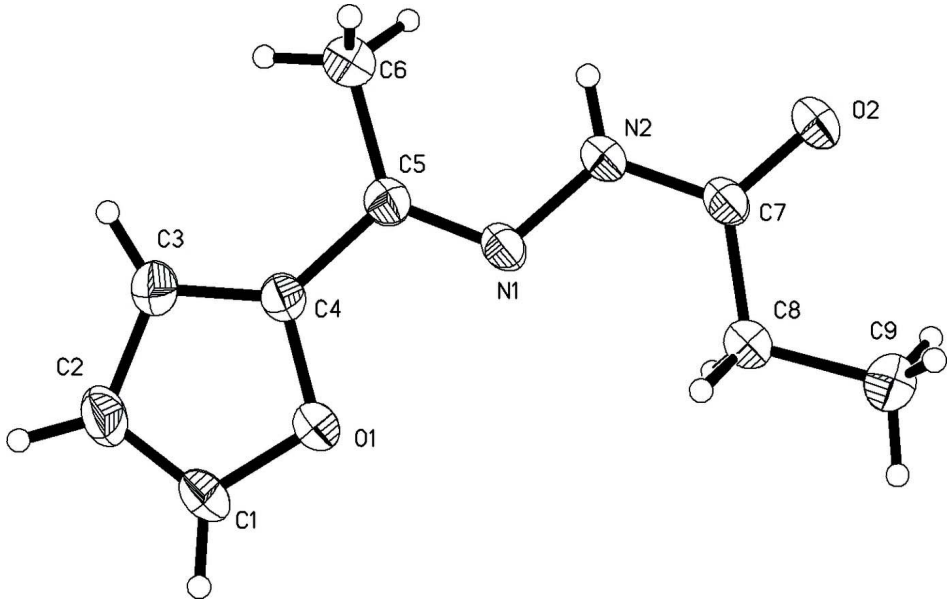

Figure 1

Structure of the title compound at 30% probability displacement ellipsoids showing the atom-numbering scheme.

N′-[1-(2-Furyl)ethenyl]propanohydrazide

Crystal data

$C_9H_{12}N_2O_2$
$M_r = 180.21$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 4.3314\ (13)$ Å
$b = 9.560\ (3)$ Å
$c = 11.695\ (4)$ Å
$\alpha = 102.338\ (6)°$
$\beta = 98.665\ (5)°$
$\gamma = 91.273\ (5)°$
$V = 466.9\ (3)$ Å^3
$Z = 2$
$F(000) = 192$
$D_x = 1.282$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 960 reflections
$\theta = 3.8–25.0°$
$\mu = 0.09$ mm^{-1}
$T = 294$ K
Rod, yellow
0.38 × 0.14 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
2708 measured reflections
1893 independent reflections
1188 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.8°$
$h = -5\rightarrow5$
$k = -11\rightarrow11$
$l = -14\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.149$
$S = 1.01$
1893 reflections
120 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.0266P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5016 (3)	0.10932 (14)	0.42113 (12)	0.0532 (4)
O2	−0.5552 (4)	−0.16062 (16)	0.03731 (13)	0.0648 (5)
N1	0.0408 (3)	0.04514 (17)	0.23834 (13)	0.0438 (4)
N2	−0.1921 (4)	0.00438 (17)	0.14220 (14)	0.0471 (4)
H2	−0.2381	0.0606	0.0945	0.057*
C1	0.7274 (5)	0.1722 (3)	0.51195 (18)	0.0590 (6)
H1	0.8264	0.1264	0.5689	0.071*
C2	0.7882 (5)	0.3074 (3)	0.50874 (19)	0.0616 (6)
H2A	0.9332	0.3725	0.5616	0.074*
C3	0.5891 (5)	0.3330 (2)	0.40919 (18)	0.0542 (6)
H3	0.5778	0.4187	0.3837	0.065*
C4	0.4190 (4)	0.2105 (2)	0.35796 (16)	0.0424 (5)
C5	0.1730 (4)	0.1706 (2)	0.25591 (16)	0.0416 (5)
C6	0.0995 (5)	0.2787 (2)	0.18300 (18)	0.0598 (6)
H6A	0.2015	0.2570	0.1144	0.090*
H6B	0.1721	0.3724	0.2291	0.090*
H6C	−0.1225	0.2766	0.1584	0.090*
C7	−0.3475 (5)	−0.1237 (2)	0.12307 (17)	0.0473 (5)
C8	−0.2606 (5)	−0.2171 (2)	0.20869 (19)	0.0579 (6)
H8A	−0.3313	−0.1758	0.2828	0.070*
H8B	−0.0345	−0.2188	0.2245	0.070*
C9	−0.3969 (7)	−0.3681 (2)	0.1651 (2)	0.0839 (8)
H9A	−0.6207	−0.3674	0.1483	0.126*
H9B	−0.3393	−0.4218	0.2249	0.126*
H9C	−0.3181	−0.4118	0.0942	0.126*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0553 (8)	0.0502 (8)	0.0480 (8)	−0.0076 (6)	−0.0124 (7)	0.0125 (7)
O2	0.0681 (10)	0.0591 (9)	0.0549 (9)	−0.0098 (7)	−0.0248 (8)	0.0106 (7)
N1	0.0404 (9)	0.0468 (9)	0.0388 (9)	−0.0009 (7)	−0.0046 (7)	0.0055 (7)

N2	0.0464 (9)	0.0467 (10)	0.0429 (9)	−0.0028 (7)	−0.0096 (7)	0.0103 (7)
C1	0.0565 (13)	0.0668 (15)	0.0453 (12)	−0.0079 (11)	−0.0145 (10)	0.0108 (10)
C2	0.0605 (14)	0.0653 (15)	0.0484 (12)	−0.0172 (11)	−0.0077 (10)	0.0029 (11)
C3	0.0579 (13)	0.0475 (12)	0.0523 (13)	−0.0093 (10)	0.0005 (10)	0.0076 (10)
C4	0.0416 (10)	0.0434 (10)	0.0402 (11)	−0.0023 (8)	0.0027 (9)	0.0078 (8)
C5	0.0393 (10)	0.0442 (11)	0.0403 (11)	0.0007 (8)	0.0054 (8)	0.0082 (8)
C6	0.0613 (14)	0.0611 (13)	0.0548 (14)	−0.0063 (11)	−0.0053 (11)	0.0191 (11)
C7	0.0474 (11)	0.0478 (12)	0.0405 (11)	0.0009 (9)	−0.0069 (9)	0.0056 (9)
C8	0.0639 (13)	0.0508 (12)	0.0528 (13)	−0.0044 (10)	−0.0118 (11)	0.0128 (10)
C9	0.0964 (19)	0.0543 (14)	0.0903 (19)	−0.0127 (13)	−0.0248 (16)	0.0214 (13)

Geometric parameters (Å, º)

O1—C1	1.354 (2)	C4—C5	1.452 (3)
O1—C4	1.361 (2)	C5—C6	1.485 (3)
O2—C7	1.226 (2)	C6—H6A	0.9600
N1—C5	1.280 (2)	C6—H6B	0.9600
N1—N2	1.374 (2)	C6—H6C	0.9600
N2—C7	1.343 (2)	C7—C8	1.492 (3)
N2—H2	0.8600	C8—C9	1.500 (3)
C1—C2	1.323 (3)	C8—H8A	0.9700
C1—H1	0.9300	C8—H8B	0.9700
C2—C3	1.410 (3)	C9—H9A	0.9600
C2—H2A	0.9300	C9—H9B	0.9600
C3—C4	1.342 (3)	C9—H9C	0.9600
C3—H3	0.9300		
C1—O1—C4	106.66 (15)	C5—C6—H6B	109.5
C5—N1—N2	117.46 (16)	H6A—C6—H6B	109.5
C7—N2—N1	119.69 (16)	C5—C6—H6C	109.5
C7—N2—H2	120.2	H6A—C6—H6C	109.5
N1—N2—H2	120.2	H6B—C6—H6C	109.5
C2—C1—O1	110.85 (19)	O2—C7—N2	119.93 (18)
C2—C1—H1	124.6	O2—C7—C8	121.89 (18)
O1—C1—H1	124.6	N2—C7—C8	118.18 (17)
C1—C2—C3	106.23 (19)	C7—C8—C9	113.33 (19)
C1—C2—H2A	126.9	C7—C8—H8A	108.9
C3—C2—H2A	126.9	C9—C8—H8A	108.9
C4—C3—C2	107.3 (2)	C7—C8—H8B	108.9
C4—C3—H3	126.4	C9—C8—H8B	108.9
C2—C3—H3	126.4	H8A—C8—H8B	107.7
C3—C4—O1	109.02 (18)	C8—C9—H9A	109.5
C3—C4—C5	133.29 (19)	C8—C9—H9B	109.5
O1—C4—C5	117.66 (16)	H9A—C9—H9B	109.5
N1—C5—C4	116.21 (17)	C8—C9—H9C	109.5
N1—C5—C6	126.62 (17)	H9A—C9—H9C	109.5
C4—C5—C6	117.16 (16)	H9B—C9—H9C	109.5
C5—C6—H6A	109.5		

C5—N1—N2—C7	−177.01 (17)	N2—N1—C5—C6	0.4 (3)
C4—O1—C1—C2	0.3 (2)	C3—C4—C5—N1	−173.8 (2)
O1—C1—C2—C3	−0.2 (3)	O1—C4—C5—N1	4.2 (3)
C1—C2—C3—C4	0.0 (3)	C3—C4—C5—C6	6.0 (3)
C2—C3—C4—O1	0.2 (2)	O1—C4—C5—C6	−176.03 (17)
C2—C3—C4—C5	178.3 (2)	N1—N2—C7—O2	−179.89 (17)
C1—O1—C4—C3	−0.3 (2)	N1—N2—C7—C8	0.4 (3)
C1—O1—C4—C5	−178.77 (16)	O2—C7—C8—C9	12.9 (3)
N2—N1—C5—C4	−179.81 (15)	N2—C7—C8—C9	−167.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.86	2.08	2.925 (2)	166

Symmetry code: (i) −*x*−1, −*y*, −*z*.