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2-(1*H*-Benzotriazol-1-yl)-*N*′-(propan-2-ylidene)acetohydrazide

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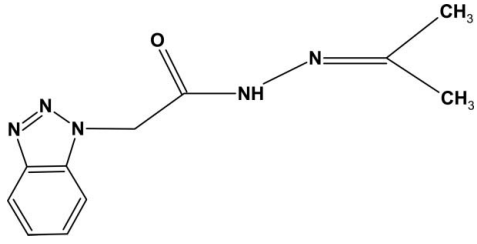
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.187; data-to-parameter ratio = 13.4.

In the title compound, $C_{11}H_{13}N_5O$, which was synthesized by the reaction of 2-(1*H*-benzotriazol-1-yl)acetohydrazide with acetone, all bond lengths and angles are normal. Weak intermolecular N—H···O hydrogen bonds link the molecules into chains running along the *c* axis.

Related literature

For related literature, see: Allen *et al.* (1987); Anderson *et al.* (1997); Garnovski *et al.* (1993); Musie *et al.* (2001); Paul *et al.* (2002); Xu *et al.* (2002).



Experimental

Crystal data

$C_{11}H_{13}N_5O$
M_r = 231.26
Monoclinic, $P2_1/c$
a = 10.841 (2) Å
b = 13.426 (3) Å
c = 8.2811 (17) Å
β = 100.737 (4)°
V = 1184.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.987, T_{max} = 0.991
6155 measured reflections
2094 independent reflections
1325 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.187
S = 1.00
2094 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O1^{i}	0.86	2.16	2.933 (2)	150

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2334).

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supplementary materials

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2-(1*H*-Benzotriazol-1-yl)-*N*'-(propan-2-ylidene)acetohydrazide

Z.-Q. Shi, N.-N. Ji, Z.-B. Zheng and J.-K. Li

Comment

In recent years, a number of Schiff-bases have been investigated in terms of their coordination chemistry (Garnovski *et al.*, 1993; Musie *et al.*, 2001; Paul *et al.*, 2002) and biological systems (Anderson *et al.*, 1997). Schiff-bases containing the triazole group have attracted much attention because they exhibit potential bioactivities (Xu *et al.*, 2002). In order to search for new triazole compounds with higher bioactivity, the title compound, (I), was synthesized and its crystal structure determined.

In (I) (Fig. 1), the bond lengths and angles are in good agreement with the expected values (Allen *et al.*, 1987). In the crystal structure, the molecules are linked into infinite chains by N—H···O hydrogen bonds (Table 1, Fig. 2).

Experimental

The 2-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)acetohydrazide (1 mmol, 191.2 mg) was added to acetone solvent (20 ml). The mixture was stirred under reflux conditions (343 K) for 3 h to give a clear solution. The solution was filtered and after a week colourless crystals suitable for X-ray diffraction study were obtained. *M*.p. 207–208 K. Analysis: calculated for $C_{11}H_{13}N_5O$: C 57.13, H 5.67, N 30.27%; found: C57.10, H 5.71, N 30.22%.

Refinement

All H atoms were placed in idealized positions (C—H = 0.93–0.97 Å, N—H = 0.86 Å) and refined as riding atoms, with U_{iso}(H) = 1.2–1.5U_{eq} of the parent atom.

Figures

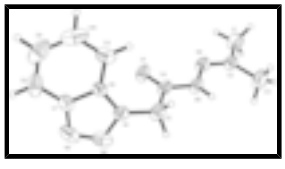

Fig. 1. The molecular structure of (I) showing the atomic numbering and displacement ellipsoids drawn at the 50% probability level.

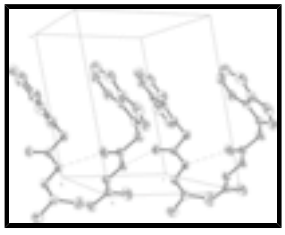

Fig. 2. A portion of the crystal packing showing the hydrogen-bonded (dashed lines) chain of the molecules. H atoms have been omitted for clarity.

2-(1*H*-Benzotriazol-1-yl)-*N*'-(propan-2-ylidene)acetohydrazide

Crystal data

$C_{11}H_{13}N_5O$	$F_{000} = 488$
$M_r = 231.26$	$D_x = 1.297$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1111 reflections
$a = 10.841$ (2) Å	$\theta = 2.4$–25.7º
$b = 13.426$ (3) Å	$\mu = 0.09$ mm^{-1}
$c = 8.2811$ (17) Å	$T = 295$ K
$\beta = 100.737$ (4)º	Block, colourless
$V = 1184.3$ (4) Å^3	0.15 × 0.12 × 0.10 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2094 independent reflections
Radiation source: fine-focus sealed tube	1325 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.030$
$T = 295$ K	$\theta_{max} = 25.1$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12\rightarrow7$
$T_{min} = 0.987$, $T_{max} = 0.991$	$k = -15\rightarrow15$
6155 measured reflections	$l = -9\rightarrow9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.187$	$w = 1/[\sigma^2(F_o^2) + (0.1178P)^2 + 0.0018P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.002$
2094 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
156 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.22589 (17)	0.83827 (14)	0.08278 (19)	0.0729 (6)
N1	0.40099 (19)	0.91461 (15)	0.3268 (2)	0.0556 (6)
N2	0.3838 (2)	1.01387 (19)	0.3451 (3)	0.0759 (7)
N3	0.4713 (3)	1.06118 (16)	0.2900 (3)	0.0789 (8)
N4	0.05295 (19)	0.70349 (16)	0.1188 (2)	0.0602 (6)
N5	0.13678 (18)	0.74222 (15)	0.2524 (2)	0.0587 (6)
H5	0.1346	0.7241	0.3514	0.070*
C1	−0.1164 (3)	0.6016 (2)	−0.0022 (4)	0.0843 (10)
H1A	−0.0926	0.6281	−0.0996	0.126*
H1B	−0.2009	0.6213	0.0016	0.126*
H1C	−0.1113	0.5302	−0.0037	0.126*
C2	−0.0295 (2)	0.6409 (2)	0.1464 (3)	0.0591 (7)
C3	−0.0470 (3)	0.6041 (3)	0.3097 (4)	0.0995 (12)
H3A	0.0069	0.5479	0.3410	0.149*
H3B	−0.1328	0.5844	0.3040	0.149*
H3C	−0.0263	0.6561	0.3898	0.149*
C4	0.2205 (2)	0.80851 (19)	0.2198 (3)	0.0550 (7)
C5	0.3128 (3)	0.8439 (2)	0.3710 (3)	0.0744 (9)
H5A	0.2669	0.8747	0.4478	0.089*
H5B	0.3581	0.7872	0.4251	0.089*
C6	0.5010 (2)	0.89849 (16)	0.2542 (3)	0.0471 (6)
C7	0.5460 (2)	0.99256 (18)	0.2310 (3)	0.0577 (7)
C8	0.6471 (4)	1.0065 (3)	0.1553 (4)	0.0903 (11)
H8	0.6770	1.0699	0.1395	0.108*
C9	0.7013 (3)	0.9248 (5)	0.1048 (4)	0.1078 (14)
H9	0.7700	0.9321	0.0533	0.129*
C10	0.6563 (4)	0.8293 (4)	0.1283 (4)	0.1016 (13)
H10	0.6956	0.7747	0.0906	0.122*
C11	0.5558 (3)	0.8132 (2)	0.2054 (3)	0.0691 (8)
H11	0.5269	0.7497	0.2234	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0772 (13)	0.1055 (15)	0.0345 (10)	−0.0323 (10)	0.0061 (8)	0.0034 (8)
N1	0.0561 (13)	0.0654 (13)	0.0429 (11)	−0.0076 (10)	0.0033 (10)	−0.0075 (9)
N2	0.0823 (18)	0.0720 (16)	0.0655 (15)	0.0156 (13)	−0.0069 (13)	−0.0223 (12)
N3	0.103 (2)	0.0483 (13)	0.0728 (17)	0.0026 (14)	−0.0159 (15)	−0.0053 (11)
N4	0.0559 (13)	0.0835 (14)	0.0378 (11)	−0.0124 (11)	0.0004 (9)	−0.0005 (9)
N5	0.0576 (13)	0.0859 (15)	0.0309 (10)	−0.0169 (11)	0.0034 (9)	0.0024 (9)
C1	0.0673 (19)	0.112 (2)	0.070 (2)	−0.0265 (16)	0.0024 (15)	−0.0121 (15)
C2	0.0534 (16)	0.0739 (17)	0.0499 (15)	−0.0065 (13)	0.0091 (12)	−0.0015 (12)
C3	0.104 (3)	0.132 (3)	0.063 (2)	−0.053 (2)	0.0172 (18)	0.0070 (17)
C4	0.0533 (15)	0.0777 (16)	0.0343 (13)	−0.0093 (13)	0.0085 (11)	−0.0025 (11)
C5	0.0662 (18)	0.114 (2)	0.0405 (14)	−0.0309 (16)	0.0047 (12)	−0.0013 (14)
C6	0.0518 (14)	0.0485 (14)	0.0371 (12)	−0.0028 (11)	−0.0020 (10)	−0.0015 (9)
C7	0.0669 (17)	0.0536 (15)	0.0470 (14)	−0.0098 (13)	−0.0037 (12)	0.0057 (11)
C8	0.088 (2)	0.118 (3)	0.0598 (19)	−0.042 (2)	−0.0013 (17)	0.0257 (18)
C9	0.069 (2)	0.197 (5)	0.057 (2)	−0.012 (3)	0.0109 (17)	0.002 (3)
C10	0.085 (3)	0.145 (4)	0.068 (2)	0.046 (2)	−0.0028 (19)	−0.034 (2)
C11	0.081 (2)	0.0591 (16)	0.0598 (17)	0.0144 (14)	−0.0050 (15)	−0.0113 (12)

Geometric parameters (Å, °)

O1—C4	1.215 (3)	C3—H3B	0.9600
N1—C6	1.352 (3)	C3—H3C	0.9600
N1—N2	1.358 (3)	C4—C5	1.526 (3)
N1—C5	1.441 (3)	C5—H5A	0.9700
N2—N3	1.293 (3)	C5—H5B	0.9700
N3—C7	1.375 (4)	C6—C7	1.380 (3)
N4—C2	1.278 (3)	C6—C11	1.384 (3)
N4—N5	1.395 (3)	C7—C8	1.373 (4)
N5—C4	1.334 (3)	C8—C9	1.347 (5)
N5—H5	0.8600	C8—H8	0.9300
C1—C2	1.500 (4)	C9—C10	1.399 (6)
C1—H1A	0.9600	C9—H9	0.9300
C1—H1B	0.9600	C10—C11	1.379 (5)
C1—H1C	0.9600	C10—H10	0.9300
C2—C3	1.485 (4)	C11—H11	0.9300
C3—H3A	0.9600		
C6—N1—N2	110.2 (2)	N5—C4—C5	114.2 (2)
C6—N1—C5	129.2 (2)	N1—C5—C4	111.2 (2)
N2—N1—C5	120.4 (2)	N1—C5—H5A	109.4
N3—N2—N1	108.5 (2)	C4—C5—H5A	109.4
N2—N3—C7	108.4 (2)	N1—C5—H5B	109.4
C2—N4—N5	118.48 (19)	C4—C5—H5B	109.4
C4—N5—N4	117.10 (18)	H5A—C5—H5B	108.0
C4—N5—H5	121.4	N1—C6—C7	104.4 (2)

N4—N5—H5	121.4	N1—C6—C11	133.3 (2)
C2—C1—H1A	109.5	C7—C6—C11	122.3 (3)
C2—C1—H1B	109.5	C8—C7—N3	130.1 (3)
H1A—C1—H1B	109.5	C8—C7—C6	121.4 (3)
C2—C1—H1C	109.5	N3—C7—C6	108.5 (2)
H1A—C1—H1C	109.5	C9—C8—C7	117.6 (3)
H1B—C1—H1C	109.5	C9—C8—H8	121.2
N4—C2—C3	126.5 (2)	C7—C8—H8	121.2
N4—C2—C1	116.0 (2)	C8—C9—C10	121.3 (3)
C3—C2—C1	117.6 (2)	C8—C9—H9	119.4
C2—C3—H3A	109.5	C10—C9—H9	119.4
C2—C3—H3B	109.5	C11—C10—C9	122.3 (3)
H3A—C3—H3B	109.5	C11—C10—H10	118.9
C2—C3—H3C	109.5	C9—C10—H10	118.9
H3A—C3—H3C	109.5	C10—C11—C6	115.1 (3)
H3B—C3—H3C	109.5	C10—C11—H11	122.4
O1—C4—N5	124.1 (2)	C6—C11—H11	122.4
O1—C4—C5	121.7 (2)		
C6—N1—N2—N3	−1.5 (3)	C5—N1—C6—C11	−3.4 (4)
C5—N1—N2—N3	−177.0 (2)	N2—N3—C7—C8	177.2 (3)
N1—N2—N3—C7	1.3 (3)	N2—N3—C7—C6	−0.7 (3)
C2—N4—N5—C4	−179.0 (2)	N1—C6—C7—C8	−178.3 (2)
N5—N4—C2—C3	0.3 (4)	C11—C6—C7—C8	1.1 (4)
N5—N4—C2—C1	−179.7 (2)	N1—C6—C7—N3	−0.2 (2)
N4—N5—C4—O1	1.7 (4)	C11—C6—C7—N3	179.2 (2)
N4—N5—C4—C5	−177.3 (2)	N3—C7—C8—C9	−178.0 (3)
C6—N1—C5—C4	−75.1 (3)	C6—C7—C8—C9	−0.2 (4)
N2—N1—C5—C4	99.4 (3)	C7—C8—C9—C10	0.1 (5)
O1—C4—C5—N1	0.5 (4)	C8—C9—C10—C11	−0.8 (5)
N5—C4—C5—N1	179.5 (2)	C9—C10—C11—C6	1.5 (4)
N2—N1—C6—C7	1.0 (2)	N1—C6—C11—C10	177.6 (2)
C5—N1—C6—C7	176.0 (2)	C7—C6—C11—C10	−1.6 (3)
N2—N1—C6—C11	−178.4 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···O1^{i}	0.86	2.16	2.933 (2)	150

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

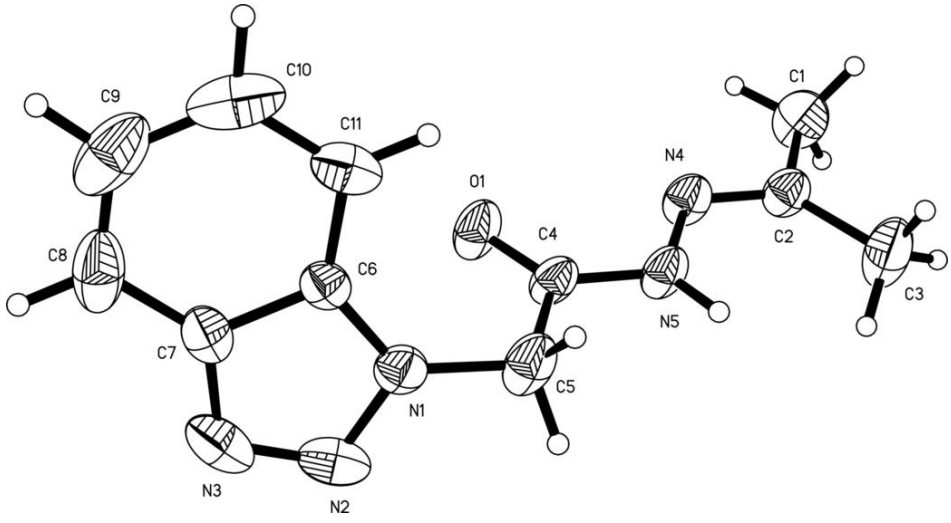

Fig. 2