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1-Benzyl-5-methyl-1*H*-1,2,3-triazole-4-carboxylic acid

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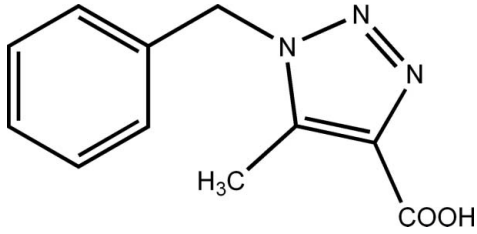
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.053; wR factor = 0.115; data-to-parameter ratio = 16.6.

In the title molecule, $C_{11}H_{11}N_3O_2$, the dihedral angle between the benzene and triazole rings is 76.47 (10)°. The crystal structure exhibits intermolecular O—H···N hydrogen bonds, which lead to the formation of helical chains along [001].

Related literature

For the synthesis of the title compound, see: El Khadem *et al.* (1968). For the biological activity of triazole compounds, see: Olesen *et al.* (2003); Tian *et al.* (2005). For related structures, see: Xiao *et al.* (2008); Lin *et al.* (2008). For structural details of a monohydrate of the title compound, see: Zhao (2009).



Experimental

Crystal data

$C_{11}H_{11}N_3O_2$
M_r = 217.23
Trigonal, $P3_1$
a = 10.1178 (7) Å
c = 8.9971 (8) Å
V = 797.64 (11) Å^3
Z = 3
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.20 × 0.18 × 0.15 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.921, T_{max} = 1.000
8294 measured reflections
2435 independent reflections
1511 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.115
S = 0.98
2435 reflections
147 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.91	2.721 (3)	171

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL/PC*.

This work was supported financially by the Southeast University Fund for Young Researchers.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LR2044).

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supporting information

Acta Cryst. (2012). E**68**, o322 [doi:10.1107/S1600536811056297]

1-Benzyl-5-methyl-1*H*-1,2,3-triazole-4-carboxylic acid

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S1. Comment

Triazole-related molecules have attracted considerable attention due to their biological activities (Olesen *et al.*, 2003; Tian *et al.*, 2005). Recently, we have reported a few triazole compounds (Lin *et al.* 2008; Xiao *et al.* 2008). As an extension of our work on the structural characterization of the triazole-related compounds, we report herein the crystal structure of the title compound (Fig. 1), a monohydrate of which has been previously reported (Zhao *et al.*, 2009) .

The dihedral angle between the benzene and tirazole rings is 76.47 (10)°. The crystal structure exhibits intermolecular O—H···N hydrogen bonds which lead to the formation of one-dimensional chains along the [001] direction (Fig. 2.; Table 1).

S2. Experimental

The title compound was prepared from azidomethylbenzene according to the reported method (El Khadem *et al.* 1968). $NiCl_2$ (1 mmol), NaN_3 (2 mmol) and the title compound (2 mmol) were placed in a thick Pyrex tube (*ca* 20 cm in length). After addition of 2.0 ml of water, the tube was frozen with liquid N_2, evacuated under vacuum, and sealed with a torch. The tube was heated at 120 °C for 3 days to give colourless prismatic crystals suitable for X-ray analysis.

S3. Refinement

All H atoms were detected in a difference map, but were placed in calculated positions and refined using a riding motion approxmation, with C—H=0.93–0.97Å and with U_{iso}(H)=1.2U_{eq}(C) or 1.5U_{eq}(C) . The bond distance O—H=0.82 Å and U_{iso}(H)=1.5U_{eq}(O).

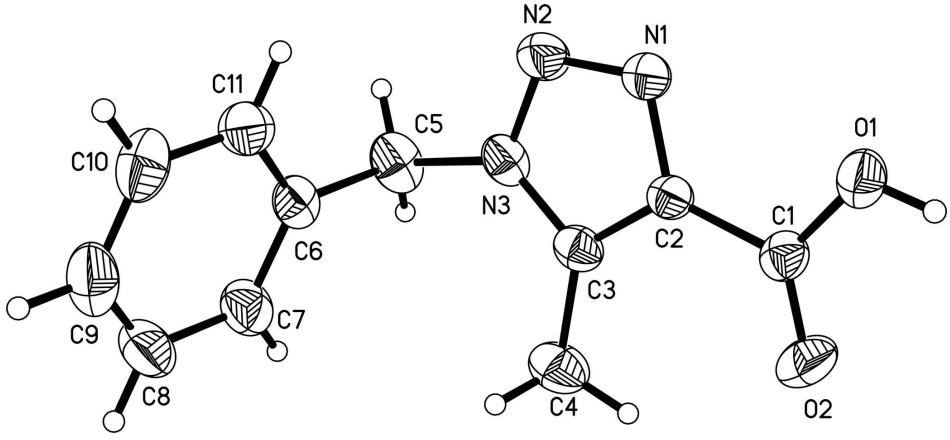

Figure 1

The molecular structure of the title compound. The displacement ellipsoids are drawn at the 30% probability level.

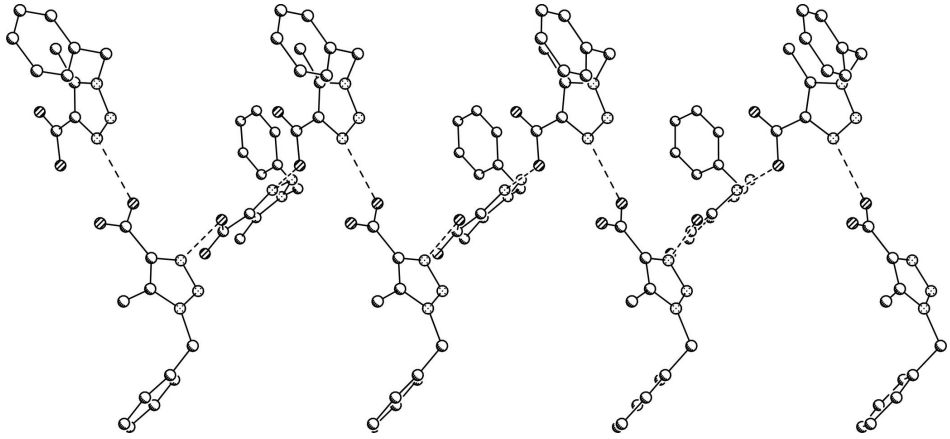

Figure 2

Diagram of the molecules linked into one dimensional chains by O—H···N hydrogen bonds.

1-Benzyl-5-methyl-1*H*-1,2,3-triazole-4-carboxylic acid

Crystal data

$C_{11}H_{11}N_3O_2$
$M_r = 217.23$
Trigonal, $P3_1$
Hall symbol: P 31
$a = 10.1178\ (7)$ Å
$c = 8.9971\ (8)$ Å
$V = 797.64\ (11)$ Å^3
$Z = 3$
$F(000) = 342$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1614 reflections
$\theta = 3.2–27.4°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Prism, colourless
0.20 × 0.18 × 0.15 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.921$, $T_{max} = 1.000$
8294 measured reflections
2435 independent reflections
1511 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.3°$
$h = -13\rightarrow12$
$k = -13\rightarrow13$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.115$
$S = 0.98$
2435 reflections
147 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5374 (3)	0.4836 (3)	−0.0739 (3)	0.0501 (7)
C2	0.4072 (3)	0.4056 (3)	0.0273 (3)	0.0440 (6)
C3	0.2816 (3)	0.4222 (3)	0.0376 (3)	0.0505 (6)
C4	0.2356 (4)	0.5194 (4)	−0.0452 (4)	0.0751 (9)
H4A	0.1509	0.4566	−0.1088	0.113*
H4B	0.3198	0.5920	−0.1042	0.113*
H4C	0.2064	0.5725	0.0239	0.113*
C5	0.0466 (3)	0.2884 (4)	0.2051 (3)	0.0709 (9)
H5A	0.0400	0.3806	0.2120	0.085*
H5B	0.0333	0.2457	0.3042	0.085*
C6	−0.0779 (3)	0.1758 (3)	0.1057 (3)	0.0545 (7)
C7	−0.1626 (4)	0.2174 (4)	0.0197 (4)	0.0715 (9)
H7	−0.1439	0.3172	0.0231	0.086*
C8	−0.2762 (4)	0.1118 (5)	−0.0726 (4)	0.0880 (11)
H8	−0.3333	0.1408	−0.1309	0.106*
C9	−0.3039 (4)	−0.0348 (4)	−0.0778 (4)	0.0846 (11)
H9	−0.3792	−0.1056	−0.1405	0.102*
C10	−0.2215 (4)	−0.0772 (4)	0.0086 (4)	0.0809 (10)
H10	−0.2417	−0.1775	0.0060	0.097*
C11	−0.1093 (4)	0.0259 (4)	0.0992 (4)	0.0675 (8)
H11	−0.0531	−0.0045	0.1573	0.081*
N1	0.3952 (3)	0.3015 (3)	0.1301 (2)	0.0558 (6)
N2	0.2667 (3)	0.2531 (3)	0.2037 (2)	0.0650 (7)
N3	0.1987 (3)	0.3270 (3)	0.1477 (2)	0.0559 (6)
O1	0.6345 (2)	0.4335 (2)	−0.0625 (2)	0.0648 (6)
H1	0.7135	0.4916	−0.1068	0.097*
O2	0.5511 (2)	0.5822 (2)	−0.1573 (2)	0.0758 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0500 (16)	0.0416 (15)	0.0522 (16)	0.0180 (13)	−0.0017 (13)	−0.0012 (13)
C2	0.0462 (15)	0.0386 (13)	0.0462 (14)	0.0204 (12)	−0.0054 (12)	−0.0015 (11)
C3	0.0554 (16)	0.0502 (16)	0.0471 (14)	0.0273 (14)	−0.0109 (14)	−0.0081 (13)
C4	0.084 (2)	0.076 (2)	0.085 (2)	0.054 (2)	−0.0121 (19)	0.0013 (18)
C5	0.0624 (19)	0.102 (2)	0.0573 (18)	0.0480 (19)	0.0045 (14)	−0.0167 (17)

C6	0.0455 (16)	0.077 (2)	0.0447 (15)	0.0331 (15)	0.0101 (13)	−0.0023 (14)
C7	0.059 (2)	0.076 (2)	0.088 (2)	0.0399 (19)	−0.0039 (18)	0.0008 (19)
C8	0.060 (2)	0.120 (3)	0.084 (2)	0.044 (2)	−0.0097 (18)	0.013 (2)
C9	0.056 (2)	0.096 (3)	0.078 (2)	0.019 (2)	0.0024 (17)	−0.012 (2)
C10	0.059 (2)	0.069 (2)	0.103 (3)	0.0232 (19)	0.018 (2)	−0.001 (2)
C11	0.061 (2)	0.079 (2)	0.070 (2)	0.0404 (18)	0.0098 (16)	0.0132 (18)
N1	0.0510 (14)	0.0652 (15)	0.0546 (14)	0.0315 (13)	0.0046 (11)	0.0118 (12)
N2	0.0598 (16)	0.087 (2)	0.0519 (14)	0.0393 (15)	0.0036 (12)	0.0153 (14)
N3	0.0499 (14)	0.0745 (16)	0.0479 (13)	0.0345 (13)	−0.0050 (11)	−0.0088 (12)
O1	0.0511 (11)	0.0661 (13)	0.0756 (14)	0.0281 (11)	0.0128 (10)	0.0121 (11)
O2	0.0828 (15)	0.0580 (13)	0.0785 (15)	0.0292 (11)	0.0135 (12)	0.0270 (12)

Geometric parameters (Å, º)

C1—O2	1.199 (3)	C6—C7	1.368 (4)
C1—O1	1.316 (3)	C6—C11	1.387 (4)
C1—C2	1.465 (4)	C7—C8	1.387 (5)
C2—N1	1.361 (3)	C7—H7	0.9300
C2—C3	1.366 (4)	C8—C9	1.366 (4)
C3—N3	1.343 (3)	C8—H8	0.9300
C3—C4	1.482 (4)	C9—C10	1.357 (5)
C4—H4A	0.9600	C9—H9	0.9300
C4—H4B	0.9600	C10—C11	1.363 (5)
C4—H4C	0.9600	C10—H10	0.9300
C5—N3	1.479 (3)	C11—H11	0.9300
C5—C6	1.500 (4)	N1—N2	1.315 (3)
C5—H5A	0.9700	N2—N3	1.342 (3)
C5—H5B	0.9700	O1—H1	0.8200
O2—C1—O1	124.8 (3)	C11—C6—C5	120.1 (3)
O2—C1—C2	122.4 (3)	C6—C7—C8	120.4 (3)
O1—C1—C2	112.8 (2)	C6—C7—H7	119.8
N1—C2—C3	108.7 (2)	C8—C7—H7	119.8
N1—C2—C1	123.2 (2)	C9—C8—C7	119.9 (3)
C3—C2—C1	128.1 (2)	C9—C8—H8	120.0
N3—C3—C2	104.3 (2)	C7—C8—H8	120.0
N3—C3—C4	123.8 (3)	C10—C9—C8	119.9 (4)
C2—C3—C4	131.9 (3)	C10—C9—H9	120.1
C3—C4—H4A	109.5	C8—C9—H9	120.1
C3—C4—H4B	109.5	C9—C10—C11	120.6 (4)
H4A—C4—H4B	109.5	C9—C10—H10	119.7
C3—C4—H4C	109.5	C11—C10—H10	119.7
H4A—C4—H4C	109.5	C10—C11—C6	120.7 (3)
H4B—C4—H4C	109.5	C10—C11—H11	119.7
N3—C5—C6	111.1 (2)	C6—C11—H11	119.7
N3—C5—H5A	109.4	N2—N1—C2	108.6 (2)
C6—C5—H5A	109.4	N1—N2—N3	106.9 (2)
N3—C5—H5B	109.4	N2—N3—C3	111.5 (2)

C6—C5—H5B	109.4	N2—N3—C5	118.5 (2)
H5A—C5—H5B	108.0	C3—N3—C5	129.9 (2)
C7—C6—C11	118.5 (3)	C1—O1—H1	109.5
C7—C6—C5	121.4 (3)		
O2—C1—C2—N1	−175.1 (3)	C9—C10—C11—C6	0.5 (5)
O1—C1—C2—N1	5.0 (4)	C7—C6—C11—C10	0.3 (4)
O2—C1—C2—C3	4.5 (4)	C5—C6—C11—C10	−179.6 (3)
O1—C1—C2—C3	−175.4 (3)	C3—C2—N1—N2	0.0 (3)
N1—C2—C3—N3	0.3 (3)	C1—C2—N1—N2	179.7 (2)
C1—C2—C3—N3	−179.4 (2)	C2—N1—N2—N3	−0.2 (3)
N1—C2—C3—C4	179.6 (3)	N1—N2—N3—C3	0.4 (3)
C1—C2—C3—C4	0.0 (5)	N1—N2—N3—C5	176.9 (2)
N3—C5—C6—C7	−109.3 (3)	C2—C3—N3—N2	−0.4 (3)
N3—C5—C6—C11	70.6 (3)	C4—C3—N3—N2	−179.9 (2)
C11—C6—C7—C8	−0.5 (5)	C2—C3—N3—C5	−176.4 (2)
C5—C6—C7—C8	179.3 (3)	C4—C3—N3—C5	4.2 (4)
C6—C7—C8—C9	0.0 (5)	C6—C5—N3—N2	−96.9 (3)
C7—C8—C9—C10	0.8 (5)	C6—C5—N3—C3	78.8 (4)
C8—C9—C10—C11	−1.0 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.91	2.721 (3)	171

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