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3-(1*H*-Benzotriazol-1-yl)-1-(4-ethylphenyl)propan-1-one

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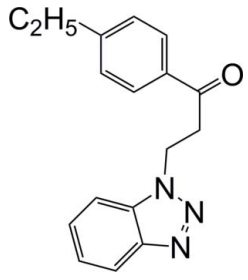
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.116; data-to-parameter ratio = 15.4.

In the molecule of the title compound, $C_{17}H_{17}N_3O$, the dihedral angle between the benzotriazole fused ring system and the other benzene ring is 70.50 (6)°. The crystal structure is stabilized by C—H···O interactions and van der Waals interactions.

Related literature

1*H*-Benzotriazole derivatives can exhibit a broad spectrum of pharmacological activities (Chen & Wu, 2005). For standard bond-length values, see Allen *et al.* (1987).



Experimental

Crystal data

$C_{17}H_{17}N_3O$
M_r = 279.34
Monoclinic, $P2_1/c$
a = 5.7577 (5) Å
b = 13.9599 (12) Å
c = 18.6746 (17) Å
β = 98.585 (5)°
V = 1484.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.22 × 0.2 × 0.1 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.983, T_{max} = 0.99
15817 measured reflections
2918 independent reflections
2410 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.05
2918 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.93	2.55	3.310 (2)	139

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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: LH2425).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Z.-Y. & Wu, M.-J. (2005). *Org. Lett.* **7**, 475–477.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

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supplementary materials

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3-(1*H*-Benzotriazol-1-yl)-1-(4-ethylphenyl)propan-1-one

W.-L. Zeng

Comment

1*H*-Benzotriazole and its derivatives are an important class of compounds because they exhibit a broad spectrum of pharmacological activities such as antifungal, antitumor and antineoplastic activities (Chen & Wu, 2005). We report here the synthesis and structure of the title compound (Fig. 1) as part of our ongoing studies of new benzotriazole compounds with potential bioactivity.

All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The benzotriazole fused rings system is essentially planar, with a dihedral angle of 0.52 (8)° between the triazole ring (atoms N1—N3/C1/C6) and the benzene ring (C1—C6). The mean plane of the benzotriazole moiety and the benzene ring (C10—C15) make a dihedral angle of 70.50 (6)°. The crystal structure (Fig. 2) is stabilized by weak C—H···O interactions and Van der Waals interactions.

Experimental

To a solution of 1-(4-ethylphenyl)-3-(dimethylamino)propan-1-one (12.05 g, 0.05 mol) in water (25 ml) was added benzotriazole (7.1 g, 0.06 mol). The mixture was heated under reflux for 5 h, yielding a copious precipitate. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a ethanol solution over a period of 6 d.

Refinement

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) and 1.5 U_{eq}(methyl C) H atoms.

Figures

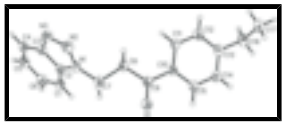

Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids.

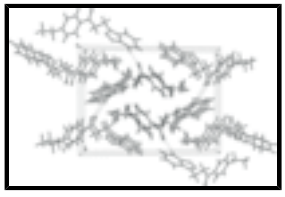

Fig. 2. The crystal packing of (I), viewed along *a* axis. Hydrogen bonds are indicated by dashed lines.

3-(1*H*-Benzotriazol-1-yl)-1-(4-ethylphenyl)propan-1-one

Crystal data

$C_{17}H_{17}N_3O$	F_{000} = 592
M_r = 279.34	D_x = 1.250 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2918 reflections
a = 5.7577 (5) Å	θ = 1.8–26º
b = 13.9599 (12) Å	μ = 0.08 mm^{-1}
c = 18.6746 (17) Å	T = 293 (2) K
β = 98.585 (5)º	Block, colourless
V = 1484.2 (2) Å^3	0.22 × 0.2 × 0.1 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2918 independent reflections
Radiation source: fine-focus sealed tube	2410 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −7→7
T_{min} = 0.983, T_{max} = 0.99	k = −16→17
15817 measured reflections	l = −18→23

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.041	$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.2889P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.116	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.05	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
2918 reflections	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
190 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0012 (2)
Secondary atom site location: difference Fourier map	

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	0.9021 (3)	0.83688 (8)	0.58482 (7)	0.0796 (4)
N1	0.5033 (2)	0.66905 (8)	0.70534 (6)	0.0481 (3)
C2	0.5548 (2)	0.62666 (9)	0.77141 (7)	0.0420 (3)
N3	0.1946 (2)	0.58572 (10)	0.71641 (7)	0.0572 (3)
C14	1.2945 (3)	0.73333 (11)	0.43061 (8)	0.0552 (4)
H14	1.4161	0.7692	0.4166	0.066*
N2	0.2864 (2)	0.64325 (10)	0.67354 (7)	0.0588 (3)
C10	0.9962 (2)	0.71539 (9)	0.50723 (7)	0.0425 (3)
C8	0.7275 (2)	0.68779 (10)	0.60405 (7)	0.0449 (3)
H8A	0.8181	0.6313	0.6206	0.054*
H8B	0.5937	0.6672	0.5697	0.054*
C9	0.8774 (2)	0.75388 (10)	0.56663 (8)	0.0472 (3)
C15	1.1769 (2)	0.76740 (10)	0.48448 (8)	0.0496 (3)
H15	1.2195	0.8262	0.5059	0.059*
C13	1.2344 (3)	0.64631 (12)	0.39706 (8)	0.0551 (4)
C4	0.3425 (3)	0.51793 (10)	0.83957 (8)	0.0532 (4)
H4	0.2099	0.4819	0.8444	0.064*
C1	0.7493 (3)	0.62898 (11)	0.82580 (8)	0.0555 (4)
H1	0.8818	0.6655	0.8217	0.067*
C3	0.3548 (2)	0.57312 (10)	0.77798 (7)	0.0440 (3)
C11	0.9337 (3)	0.62869 (11)	0.47349 (8)	0.0544 (4)
H11	0.8128	0.5926	0.4878	0.065*
C6	0.7332 (3)	0.57433 (13)	0.88542 (9)	0.0641 (4)
H6	0.8591	0.5735	0.9229	0.077*
C5	0.5333 (3)	0.51930 (12)	0.89225 (8)	0.0607 (4)
H5	0.5314	0.4829	0.9338	0.073*
C16	1.3579 (3)	0.60998 (14)	0.33634 (9)	0.0731 (5)
H16A	1.5070	0.6428	0.3380	0.088*
H16B	1.3899	0.5421	0.3432	0.088*
C7	0.6410 (3)	0.73464 (11)	0.66774 (8)	0.0577 (4)
H7A	0.7745	0.7573	0.7013	0.069*
H7B	0.5452	0.7897	0.6510	0.069*
C12	1.0502 (3)	0.59550 (12)	0.41861 (9)	0.0618 (4)

H12	1.0037	0.5379	0.3958	0.074*
C17	1.2147 (4)	0.62537 (15)	0.26425 (10)	0.0771 (5)
H17A	1.2989	0.6020	0.2272	0.116*
H17B	1.1842	0.6926	0.2571	0.116*
H17C	1.0687	0.5915	0.2619	0.116*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1232 (11)	0.0449 (6)	0.0840 (9)	−0.0106 (6)	0.0590 (8)	−0.0120 (6)
N1	0.0512 (7)	0.0521 (7)	0.0431 (6)	−0.0045 (5)	0.0134 (5)	0.0003 (5)
C2	0.0437 (7)	0.0438 (7)	0.0407 (7)	0.0027 (5)	0.0137 (5)	−0.0045 (6)
N3	0.0505 (7)	0.0662 (8)	0.0539 (7)	−0.0089 (6)	0.0046 (6)	0.0044 (6)
C14	0.0526 (8)	0.0623 (9)	0.0535 (8)	−0.0032 (7)	0.0174 (7)	0.0051 (7)
N2	0.0567 (7)	0.0695 (8)	0.0488 (7)	−0.0058 (6)	0.0031 (6)	0.0045 (6)
C10	0.0486 (7)	0.0412 (7)	0.0386 (7)	0.0026 (5)	0.0097 (5)	0.0030 (5)
C8	0.0454 (7)	0.0465 (7)	0.0440 (7)	0.0009 (6)	0.0108 (6)	0.0003 (6)
C9	0.0570 (8)	0.0412 (8)	0.0452 (7)	0.0028 (6)	0.0137 (6)	0.0019 (6)
C15	0.0552 (8)	0.0459 (8)	0.0486 (8)	−0.0045 (6)	0.0107 (6)	0.0000 (6)
C13	0.0589 (9)	0.0618 (9)	0.0465 (8)	0.0112 (7)	0.0143 (7)	0.0034 (7)
C4	0.0613 (9)	0.0470 (8)	0.0552 (9)	−0.0001 (6)	0.0216 (7)	0.0024 (6)
C1	0.0442 (8)	0.0654 (9)	0.0571 (9)	−0.0005 (7)	0.0082 (7)	−0.0079 (7)
C3	0.0442 (7)	0.0443 (7)	0.0452 (7)	−0.0004 (5)	0.0120 (6)	−0.0028 (6)
C11	0.0622 (9)	0.0499 (8)	0.0549 (8)	−0.0089 (7)	0.0209 (7)	−0.0053 (7)
C6	0.0625 (10)	0.0759 (11)	0.0506 (9)	0.0130 (8)	−0.0017 (7)	−0.0022 (8)
C5	0.0803 (11)	0.0581 (9)	0.0458 (8)	0.0148 (8)	0.0163 (7)	0.0082 (7)
C16	0.0795 (12)	0.0811 (12)	0.0638 (11)	0.0194 (9)	0.0275 (9)	−0.0006 (9)
C7	0.0739 (10)	0.0502 (8)	0.0550 (9)	−0.0078 (7)	0.0298 (8)	−0.0002 (7)
C12	0.0793 (11)	0.0517 (9)	0.0576 (9)	−0.0035 (8)	0.0206 (8)	−0.0125 (7)
C17	0.0878 (13)	0.0887 (13)	0.0602 (10)	−0.0042 (10)	0.0281 (9)	−0.0035 (9)

Geometric parameters (Å, °)

O1—C9	1.2098 (17)	C13—C16	1.513 (2)
N1—N2	1.3491 (17)	C4—C5	1.361 (2)
N1—C2	1.3606 (17)	C4—C3	1.395 (2)
N1—C7	1.4582 (17)	C4—H4	0.9300
C2—C3	1.3934 (18)	C1—C6	1.364 (2)
C2—C1	1.396 (2)	C1—H1	0.9300
N3—N2	1.3006 (18)	C11—C12	1.386 (2)
N3—C3	1.3739 (18)	C11—H11	0.9300
C14—C15	1.378 (2)	C6—C5	1.405 (2)
C14—C13	1.387 (2)	C6—H6	0.9300
C14—H14	0.9300	C5—H5	0.9300
C10—C15	1.3866 (19)	C16—C17	1.485 (3)
C10—C11	1.387 (2)	C16—H16A	0.9700
C10—C9	1.4880 (18)	C16—H16B	0.9700
C8—C9	1.5046 (18)	C7—H7A	0.9700
C8—C7	1.5058 (18)	C7—H7B	0.9700

C8—H8A	0.9700	C12—H12	0.9300
C8—H8B	0.9700	C17—H17A	0.9600
C15—H15	0.9300	C17—H17B	0.9600
C13—C12	1.385 (2)	C17—H17C	0.9600
?···?	?		
N2—N1—C2	110.20 (11)	C2—C1—H1	122.1
N2—N1—C7	119.33 (12)	N3—C3—C2	108.55 (12)
C2—N1—C7	130.47 (13)	N3—C3—C4	130.56 (13)
N1—C2—C3	104.00 (12)	C2—C3—C4	120.89 (13)
N1—C2—C1	133.85 (13)	C12—C11—C10	120.41 (14)
C3—C2—C1	122.16 (13)	C12—C11—H11	119.8
N2—N3—C3	108.09 (11)	C10—C11—H11	119.8
C15—C14—C13	121.01 (13)	C1—C6—C5	122.44 (15)
C15—C14—H14	119.5	C1—C6—H6	118.8
C13—C14—H14	119.5	C5—C6—H6	118.8
N3—N2—N1	109.17 (11)	C4—C5—C6	121.71 (14)
C15—C10—C11	118.26 (12)	C4—C5—H5	119.1
C15—C10—C9	119.27 (12)	C6—C5—H5	119.1
C11—C10—C9	122.46 (12)	C17—C16—C13	111.81 (15)
C9—C8—C7	112.38 (11)	C17—C16—H16A	109.3
C9—C8—H8A	109.1	C13—C16—H16A	109.3
C7—C8—H8A	109.1	C17—C16—H16B	109.3
C9—C8—H8B	109.1	C13—C16—H16B	109.3
C7—C8—H8B	109.1	H16A—C16—H16B	107.9
H8A—C8—H8B	107.9	N1—C7—C8	112.05 (12)
O1—C9—C10	120.48 (13)	N1—C7—H7A	109.2
O1—C9—C8	120.57 (12)	C8—C7—H7A	109.2
C10—C9—C8	118.95 (11)	N1—C7—H7B	109.2
C14—C15—C10	121.05 (13)	C8—C7—H7B	109.2
C14—C15—H15	119.5	H7A—C7—H7B	107.9
C10—C15—H15	119.5	C13—C12—C11	121.33 (15)
C12—C13—C14	117.89 (13)	C13—C12—H12	119.3
C12—C13—C16	120.80 (15)	C11—C12—H12	119.3
C14—C13—C16	121.24 (15)	C16—C17—H17A	109.5
C5—C4—C3	116.95 (14)	C16—C17—H17B	109.5
C5—C4—H4	121.5	H17A—C17—H17B	109.5
C3—C4—H4	121.5	C16—C17—H17C	109.5
C6—C1—C2	115.85 (14)	H17A—C17—H17C	109.5
C6—C1—H1	122.1	H17B—C17—H17C	109.5
N2—N1—C2—C3	−0.01 (14)	N2—N3—C3—C4	−179.29 (14)
C7—N1—C2—C3	179.27 (13)	N1—C2—C3—N3	−0.04 (14)
N2—N1—C2—C1	−179.61 (15)	C1—C2—C3—N3	179.62 (13)
C7—N1—C2—C1	−0.3 (2)	N1—C2—C3—C4	179.40 (12)
C3—N3—N2—N1	−0.08 (16)	C1—C2—C3—C4	−0.9 (2)
C2—N1—N2—N3	0.05 (16)	C5—C4—C3—N3	179.43 (14)
C7—N1—N2—N3	−179.32 (12)	C5—C4—C3—C2	0.1 (2)
C15—C10—C9—O1	15.1 (2)	C15—C10—C11—C12	0.1 (2)
C11—C10—C9—O1	−165.09 (16)	C9—C10—C11—C12	−179.69 (14)

C15—C10—C9—C8	−164.43 (13)	C2—C1—C6—C5	−0.3 (2)
C11—C10—C9—C8	15.4 (2)	C3—C4—C5—C6	0.5 (2)
C7—C8—C9—O1	−5.6 (2)	C1—C6—C5—C4	−0.5 (3)
C7—C8—C9—C10	173.93 (13)	C12—C13—C16—C17	75.6 (2)
C13—C14—C15—C10	0.6 (2)	C14—C13—C16—C17	−101.4 (2)
C11—C10—C15—C14	−1.1 (2)	N2—N1—C7—C8	−71.69 (17)
C9—C10—C15—C14	178.70 (13)	C2—N1—C7—C8	109.09 (16)
C15—C14—C13—C12	1.0 (2)	C9—C8—C7—N1	−177.86 (12)
C15—C14—C13—C16	178.11 (14)	C14—C13—C12—C11	−2.0 (2)
N1—C2—C1—C6	−179.46 (14)	C16—C13—C12—C11	−179.12 (15)
C3—C2—C1—C6	1.0 (2)	C10—C11—C12—C13	1.5 (3)
N2—N3—C3—C2	0.07 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.93	2.55	3.310 (2)	139

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

Fig. 1

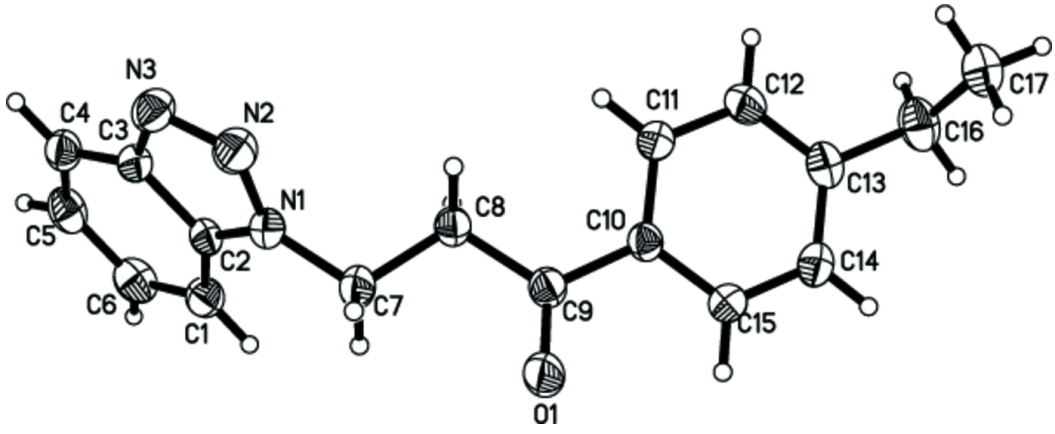
N3
C4
C3
N2
C5
N1
C8
C10
C11
C12
C17
C16
C13
C2
C14
C6
C7
C9
C1
C15
O1

Fig. 2