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

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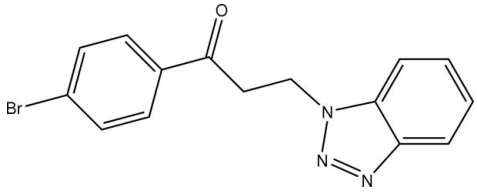
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.073; data-to-parameter ratio = 13.3.

In the molecule of the title compound, $C_{15}H_{12}BrN_3O$, the dihedral angle between the benzotriazole ring system and the benzene ring is 19.0 (1)°. π–π interactions stabilize the crystal structure (centroid-to-centroid distances of 3.729 and 3.690 Å).

Related literature

For a related structure, see: Wan *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{12}BrN_3O$
M_r = 330.18
Triclinic, $P\overline{1}$
a = 7.2310 (8) Å
b = 8.1517 (9) Å
c = 12.5240 (14) Å
α = 101.671 (2)°
β = 101.197 (1)°
γ = 105.443 (2)°
V = 672.37 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.06 mm^{-1}
T = 298 (2) K
0.29 × 0.22 × 0.19 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.443, T_{max} = 0.559
3771 measured reflections
2563 independent reflections
2232 reflections with $I > 2\sigma(I)$
R_{int} = 0.011

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.073
S = 1.06
2563 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2298).

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  doi:10.1107/S1600536807035441

supplementary materials

Acta Cryst. (2007). E**63**, o3602 [**doi:10.1107/S1600536807035441**]

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

N.-N. Tian, S. Bi, L.-L. Xu and J. Wan

Comment

Recently we have reported the strucure of 3-(1*H*-benzotriazol-1-yl)-1-(4-chloro- phenyl)-propan-1-one (Wan *et al.*, 2006). As part of a search for new benzo- triazole compounds with higher bioactivity, the title compound, (I), was synthesized and its structure is presented here.

In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The benzotriazole ring system is essentially planar, with a dihedral angle of 0.35 (1)° between the A (N1—N3/C10/C11) and B (C10—C15) rings. The mean planes of the benzotriazole ring system and the C (C1—C6) benzene ring make a dihedral angle of 19.0 (1)°.

The crystal packing is stabilized by π-π interactions involving the benzotriazole rings, with $Cg1\cdots Cg3^{i}$ [symmetry code: (i) $-x, -2-y, 1-z$] and $Cg2\cdots Cg2^{ii}$ [symmetry code: (ii) $1-x, -1-y, -z$] distances of 3.729 and 3.690 Å, where *Cg*1, *Cg*2 and *Cg*3 denote the centroids of the A, C and B rings, respectively.

Experimental

The title compound was prepared according to the literature method (Wan *et al.*, 2006). Single crystals suitable for X-ray diffracion were obtained by slow evaporation of a dichloromethane-cyclohexane (1:2 *v*/*v*) solution at room temperature over a period of one week.

Refinement

H atoms were located in difference syntheses with C—H = 0.9294–0.9301 Å and 0.9690–1.0155 Å, for aromatic and methylene H atoms, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

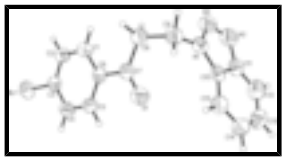

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

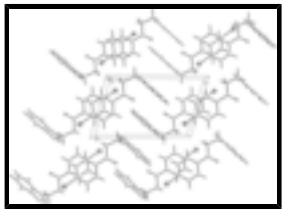

Fig. 2. A packing diagram of (I), viewed down the *a* axis.

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

Crystal data

$C_{15}H_{12}BrN_3O$	$Z = 2$
$M_r = 330.18$	$F_{000} = 332$
Triclinic, $P\overline{1}$	$D_x = 1.631$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.2310$ (8) Å	Cell parameters from 2068 reflections
$b = 8.1517$ (9) Å	$\theta = 3.0$–26.0º
$c = 12.5240$ (14) Å	$\mu = 3.06$ mm^{-1}
$\alpha = 101.671$ (2)º	$T = 298$ (2) K
$\beta = 101.197$ (1)º	Block, colourless
$\gamma = 105.443$ (2)º	0.29 × 0.22 × 0.19 mm
$V = 672.37$ (13) Å^3	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2563 independent reflections
Radiation source: fine-focus sealed tube	2232 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.011$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.0$º
$T = 298(2)$ K	$\theta_{min} = 1.7$º
ω scans	$h = -8 \rightarrow 8$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -9 \rightarrow 10$
$T_{min} = 0.443$, $T_{max} = 0.559$	$l = -15 \rightarrow 11$
3771 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.028$	H-atom parameters constrained
$wR(F^2) = 0.073$	$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.1157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
2563 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
193 parameters	$\Delta\rho_{min} = -0.29$ 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}
Br1	0.28029 (3)	−0.23329 (3)	−0.11369 (2)	0.05799 (11)
O2	0.3769 (3)	−0.6149 (2)	0.32203 (14)	0.0613 (4)
N1	0.0217 (3)	−0.9405 (2)	0.32633 (15)	0.0457 (4)
N2	−0.1692 (3)	−1.0275 (3)	0.26609 (17)	0.0558 (5)
N3	−0.2874 (3)	−0.9779 (3)	0.32235 (18)	0.0589 (5)
C1	0.2135 (3)	−0.6601 (3)	0.0221 (2)	0.0503 (5)
H1A	0.1607	−0.7824	−0.0050	0.073 (8)*
C2	0.2099 (3)	−0.5576 (3)	−0.05288 (19)	0.0514 (5)
H2A	0.1554	−0.6106	−0.1299	0.077 (9)*
C3	0.2880 (3)	−0.3772 (3)	−0.01208 (18)	0.0430 (5)
C4	0.3753 (3)	−0.2969 (3)	0.10188 (19)	0.0471 (5)
H4A	0.4315	−0.1748	0.1282	0.055 (7)*
C5	0.3773 (3)	−0.4006 (3)	0.17583 (19)	0.0448 (5)
H5A	0.4350	−0.3473	0.2525	0.056 (7)*
C6	0.2948 (3)	−0.5835 (3)	0.13774 (18)	0.0411 (5)
C7	0.2992 (3)	−0.6880 (3)	0.22262 (19)	0.0446 (5)
C8	0.2046 (4)	−0.8864 (3)	0.1827 (2)	0.0505 (5)
H8A	0.2851	−0.9369	0.1410	0.057 (7)*
H8B	0.0746	−0.9146	0.1316	0.059 (7)*
C9	0.1821 (4)	−0.9721 (3)	0.2790 (2)	0.0524 (5)
H9A	0.1653	−1.0996	0.2524	0.067 (8)*
H9B	0.3119	−0.9249	0.3407	0.052 (7)*
C10	0.0277 (3)	−0.8309 (3)	0.42539 (18)	0.0423 (5)
C11	−0.1714 (3)	−0.8559 (3)	0.42249 (19)	0.0482 (5)
C12	−0.2241 (4)	−0.7626 (4)	0.5121 (2)	0.0611 (6)
H12A	−0.3564	−0.7784	0.5115	0.061 (7)*
C13	−0.0732 (4)	−0.6475 (4)	0.6006 (2)	0.0613 (6)
H13A	−0.1040	−0.5826	0.6608	0.073 (8)*
C14	0.1265 (4)	−0.6244 (3)	0.6022 (2)	0.0581 (6)
H14A	0.2248	−0.5461	0.6646	0.070 (8)*
C15	0.1821 (3)	−0.7127 (3)	0.51643 (19)	0.0507 (5)
H15A	0.3150	−0.6956	0.5179	0.063 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.05417 (16)	0.06219 (18)	0.06435 (18)	0.01952 (12)	0.01661 (12)	0.02925 (12)
O2	0.0661 (11)	0.0559 (10)	0.0493 (10)	0.0036 (8)	0.0094 (8)	0.0133 (8)
N1	0.0457 (10)	0.0418 (9)	0.0487 (10)	0.0109 (8)	0.0123 (8)	0.0144 (8)
N2	0.0493 (11)	0.0533 (11)	0.0540 (11)	0.0051 (9)	0.0076 (9)	0.0117 (9)
N3	0.0442 (11)	0.0648 (13)	0.0596 (13)	0.0081 (10)	0.0077 (10)	0.0173 (10)
C1	0.0532 (13)	0.0382 (11)	0.0496 (13)	0.0046 (10)	0.0132 (10)	0.0035 (9)
C2	0.0534 (13)	0.0493 (13)	0.0418 (12)	0.0064 (10)	0.0098 (10)	0.0067 (10)
C3	0.0366 (10)	0.0483 (12)	0.0481 (12)	0.0152 (9)	0.0150 (9)	0.0158 (9)
C4	0.0458 (12)	0.0379 (11)	0.0543 (13)	0.0114 (9)	0.0133 (10)	0.0072 (9)
C5	0.0420 (11)	0.0440 (11)	0.0432 (12)	0.0120 (9)	0.0104 (9)	0.0039 (9)
C6	0.0349 (10)	0.0437 (11)	0.0455 (12)	0.0129 (9)	0.0151 (9)	0.0088 (9)
C7	0.0383 (11)	0.0465 (12)	0.0487 (13)	0.0113 (9)	0.0162 (9)	0.0102 (10)
C8	0.0562 (14)	0.0446 (12)	0.0559 (13)	0.0191 (11)	0.0224 (11)	0.0131 (10)
C9	0.0576 (14)	0.0461 (12)	0.0626 (14)	0.0225 (11)	0.0230 (12)	0.0194 (11)
C10	0.0434 (11)	0.0423 (11)	0.0452 (12)	0.0134 (9)	0.0118 (9)	0.0205 (9)
C11	0.0426 (11)	0.0540 (13)	0.0516 (13)	0.0152 (10)	0.0120 (10)	0.0229 (10)
C12	0.0511 (14)	0.0776 (17)	0.0674 (16)	0.0289 (13)	0.0230 (12)	0.0287 (14)
C13	0.0735 (17)	0.0673 (16)	0.0539 (14)	0.0326 (14)	0.0254 (13)	0.0181 (12)
C14	0.0617 (15)	0.0608 (15)	0.0455 (13)	0.0138 (12)	0.0087 (11)	0.0133 (11)
C15	0.0423 (12)	0.0592 (14)	0.0475 (13)	0.0124 (10)	0.0068 (10)	0.0172 (11)

Geometric parameters (Å, °)

Br1—C3	1.900 (2)	C6—C7	1.491 (3)
O2—C7	1.213 (3)	C7—C8	1.512 (3)
N1—N2	1.355 (3)	C8—C9	1.524 (3)
N1—C10	1.360 (3)	C8—H8A	0.9691
N1—C9	1.458 (3)	C8—H8B	0.9690
N2—N3	1.301 (3)	C9—H9A	0.9915
N3—C11	1.381 (3)	C9—H9B	1.0155
C1—C2	1.379 (3)	C10—C11	1.391 (3)
C1—C6	1.393 (3)	C10—C15	1.401 (3)
C1—H1A	0.9296	C11—C12	1.399 (4)
C2—C3	1.373 (3)	C12—C13	1.365 (4)
C2—H2A	0.9301	C12—H12A	0.9294
C3—C4	1.384 (3)	C13—C14	1.402 (4)
C4—C5	1.375 (3)	C13—H13A	0.9298
C4—H4A	0.9301	C14—C15	1.357 (3)
C5—C6	1.391 (3)	C14—H14A	0.9296
C5—H5A	0.9298	C15—H15A	0.9295
N2—N1—C10	110.28 (18)	C9—C8—H8A	108.7
N2—N1—C9	119.08 (19)	C7—C8—H8B	109.1
C10—N1—C9	130.63 (19)	C9—C8—H8B	108.9
N3—N2—N1	109.04 (18)	H8A—C8—H8B	107.7

N2—N3—C11	107.97 (19)	N1—C9—C8	111.96 (19)
C2—C1—C6	121.1 (2)	N1—C9—H9A	112.6
C2—C1—H1A	119.5	C8—C9—H9A	109.3
C6—C1—H1A	119.5	N1—C9—H9B	109.6
C3—C2—C1	119.0 (2)	C8—C9—H9B	109.6
C3—C2—H2A	120.9	H9A—C9—H9B	103.3
C1—C2—H2A	120.1	N1—C10—C11	104.11 (19)
C2—C3—C4	121.4 (2)	N1—C10—C15	133.9 (2)
C2—C3—Br1	119.67 (17)	C11—C10—C15	122.0 (2)
C4—C3—Br1	118.90 (16)	N3—C11—C10	108.6 (2)
C5—C4—C3	119.0 (2)	N3—C11—C12	131.0 (2)
C5—C4—H4A	120.4	C10—C11—C12	120.4 (2)
C3—C4—H4A	120.7	C13—C12—C11	117.4 (2)
C4—C5—C6	121.1 (2)	C13—C12—H12A	121.2
C4—C5—H5A	119.3	C11—C12—H12A	121.4
C6—C5—H5A	119.6	C12—C13—C14	121.4 (2)
C5—C6—C1	118.4 (2)	C12—C13—H13A	119.2
C5—C6—C7	118.38 (19)	C14—C13—H13A	119.4
C1—C6—C7	123.24 (19)	C15—C14—C13	122.5 (2)
O2—C7—C6	120.5 (2)	C15—C14—H14A	118.7
O2—C7—C8	120.5 (2)	C13—C14—H14A	118.7
C6—C7—C8	118.92 (19)	C14—C15—C10	116.2 (2)
C7—C8—C9	113.2 (2)	C14—C15—H15A	121.9
C7—C8—H8A	109.1	C10—C15—H15A	121.9
C10—N1—N2—N3	0.2 (2)	C10—N1—C9—C8	−105.7 (3)
C9—N1—N2—N3	−178.81 (19)	C7—C8—C9—N1	74.2 (3)
N1—N2—N3—C11	−0.3 (3)	N2—N1—C10—C11	0.0 (2)
C6—C1—C2—C3	0.0 (4)	C9—N1—C10—C11	178.9 (2)
C1—C2—C3—C4	2.0 (3)	N2—N1—C10—C15	−179.5 (2)
C1—C2—C3—Br1	−178.90 (17)	C9—N1—C10—C15	−0.6 (4)
C2—C3—C4—C5	−2.2 (3)	N2—N3—C11—C10	0.4 (3)
Br1—C3—C4—C5	178.65 (16)	N2—N3—C11—C12	179.9 (3)
C3—C4—C5—C6	0.5 (3)	N1—C10—C11—N3	−0.2 (2)
C4—C5—C6—C1	1.4 (3)	C15—C10—C11—N3	179.3 (2)
C4—C5—C6—C7	−179.08 (19)	N1—C10—C11—C12	−179.8 (2)
C2—C1—C6—C5	−1.6 (3)	C15—C10—C11—C12	−0.2 (3)
C2—C1—C6—C7	178.9 (2)	N3—C11—C12—C13	−179.3 (3)
C5—C6—C7—O2	−1.6 (3)	C10—C11—C12—C13	0.2 (4)
C1—C6—C7—O2	177.9 (2)	C11—C12—C13—C14	−0.3 (4)
C5—C6—C7—C8	178.20 (19)	C12—C13—C14—C15	0.6 (4)
C1—C6—C7—C8	−2.3 (3)	C13—C14—C15—C10	−0.6 (4)
O2—C7—C8—C9	11.6 (3)	N1—C10—C15—C14	179.8 (2)
C6—C7—C8—C9	−168.27 (19)	C11—C10—C15—C14	0.4 (3)
N2—N1—C9—C8	73.1 (3)		

Fig. 1

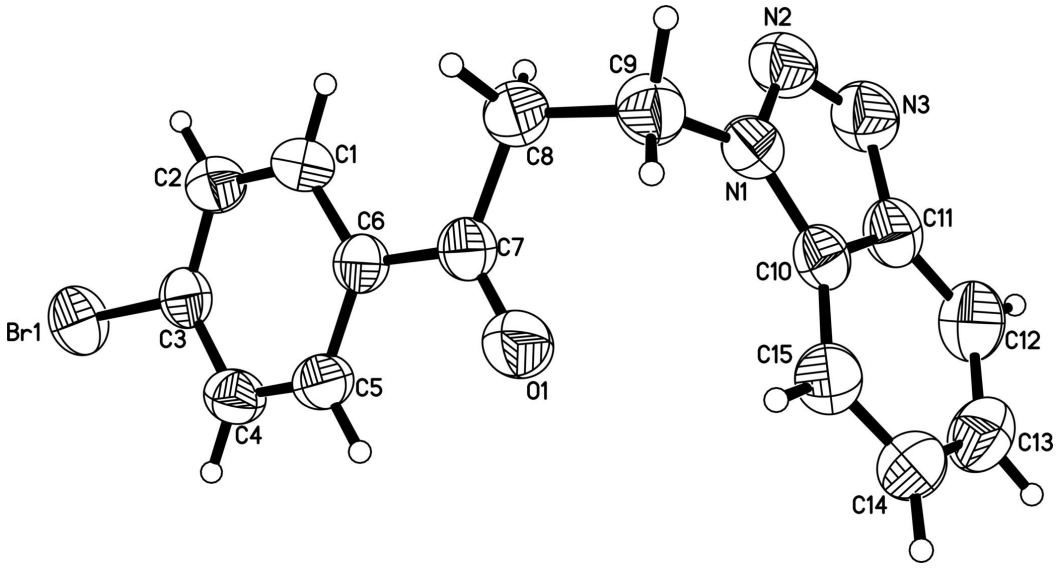

Fig. 2