Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.122
Data-to-parameter ratio = 13.7

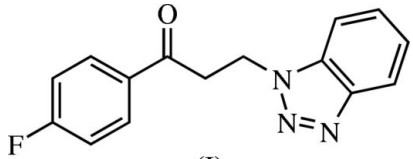
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 27 July 2006
Accepted 21 August 2006

In the title compound, $C_{15}H_{12}FN_3O$, the dihedral angle between the benzotriazole fragment and the benzene ring is 19.0 (1)°. C—H···π interactions and van der Waals forces stabilize the crystal structure.

Comment

1*H*-Benzotriazole and its derivatives exhibit a broad spectrum of pharmacological activities such as antifungal, antitumor and antineoplastic activities (Chen *et al.*, 2005). As a part of our search for new benzotriazole compounds with higher bioactivity, the title compound, (I), has been synthesized and its crystal structure is presented here.



(I)

The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The mean planes of the benzotriazole fragment and the C1–C6 benzene ring make a dihedral angle of 19.0 (1)°. The crystal packing (Fig. 2) is stabilized by C—H···π interactions (Table 1) and van der Waals forces.

Experimental

To a solution of 1-(4-fluorophenyl)-3-(dimethylamino)propan-1-one (9.8 g, 0.05 mol) in water (25 ml), benzotriazole (7.1 g, 0.06 mol) was added. The mixture was heated under reflux for 6 h, yielding a copious precipitate. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a dichloromethane–cyclohexane (1:2 *v*/*v*) solution over a period of 5 d.

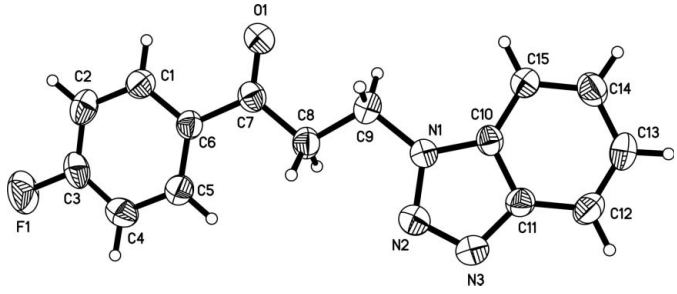


Figure 1
View of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

Crystal data

$C_{15}H_{12}FN_3O$
M_r = 269.28
Monoclinic, $P2_1/c$
a = 5.9177 (14) Å
b = 7.2815 (17) Å
c = 29.518 (7) Å
β = 96.776 (5)°
V = 1263.0 (5) Å^3
Z = 4
D_x = 1.416 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Needle, colourless
0.35 × 0.09 × 0.07 mm

Data collection

Siemens SMART 1000 CCD area detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.993
6744 measured reflections
2487 independent reflections
1584 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.122
S = 1.04
2487 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.0392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···$Cg1^{i}$	0.93	2.98	3.593 (2)	125
C15—H15A···$Cg1^{ii}$	0.93	2.87	3.491 (2)	125
C1—H1A···$Cg2^{ii}$	0.93	2.89	3.550 (2)	129

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$. $Cg1$ and $Cg2$ denote the centroids of the C1—C6 and C10—C15 rings, respectively.

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).

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).

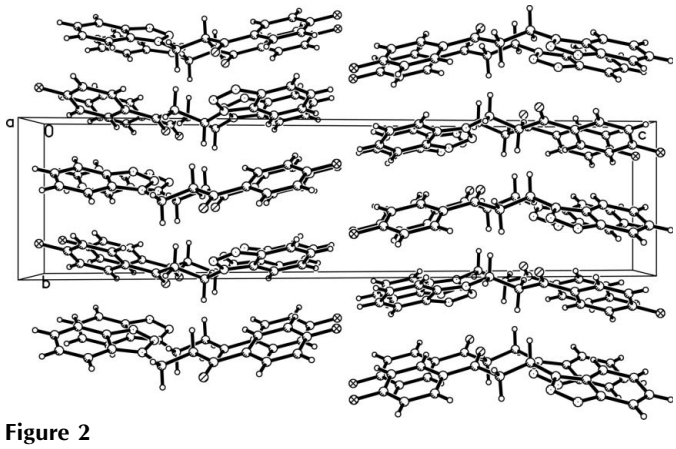


Figure 2
Packing diagram of (I), viewed down the *a* axis.

This work was supported by the Special Project of Qingdao for Leadership of Science and Technology (No. 05–2-JC-80) and the Outstanding Adult-Young Scientific Research Encouraging Foundation of Shandong Province (No. 2005BS04007).

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