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3-(1*H*-1,2,3-Benzotriazol-1-yl)-1-(4-methoxyphenyl)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 = 0.042
wR factor = 0.115
Data-to-parameter ratio = 15.0

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

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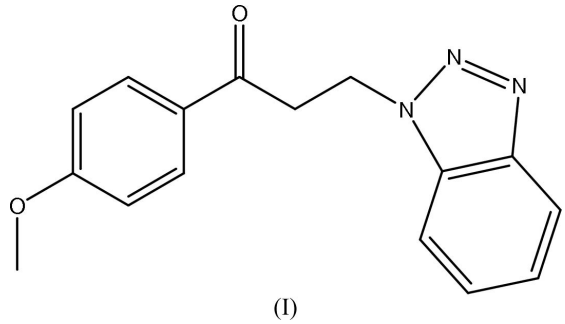
In the title compound, $C_{16}H_{15}N_3O_2$, the dihedral angle between the benzotriazole moiety and the other benzene ring is 74.40 (7)°. The short distance [3.488 (3) Å] between the centroids of benzene rings of neighbouring molecules may indicate a π–π interaction, forming centrosymmetric dimers. The packing is further stabilized by van der Waals forces.

Comment

In the framework of our study of triazole compounds, the title compound, (I) (Fig. 1), was obtained in the reaction of benzotriazole and 3-(dimethylamino)-1-(4-methoxyphenyl)-propan-1-one. We report here its crystal structure.



(I)

All bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987) and comparable with those in 1-(4-methoxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one (Wan *et al.*, 2005). The benzotriazole moiety is essentially planar; the dihedral angle between the C1–C6 and triazole rings is 0.62 (1)°. The mean plane of benzotriazole and the C10–C15 benzene ring make a dihedral angle of 74.40 (7)°. The short distance between the centroids (*Cg*) of neighbouring C10–C15 benzene rings [$Cg\cdots Cg^{i}$ = 3.488 (3) Å; symmetry code: (i) $1-x, 1-y, 1-z$] may indicate a π–π

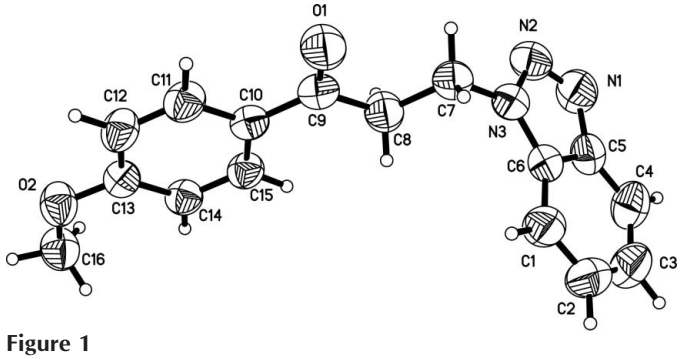


Figure 1
View of (I), showing 50% probability displacement ellipsoids and the atom-labelling scheme.

interaction, forming centrosymmetric dimers. The packing is further stabilized by van der Waals forces.

Experimental

To a solution of Mannich base 3-(dimethylamino)-1-(4-methoxyphenyl)propan-1-one (20.7 g, 0.1 mol) in water (100 ml) was added benzotriazole (11.9 g, 0.1 mol). The mixture was heated under reflux for 4 h, yielding quantities of precipitate. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a dichloromethane and cyclohexane (2:1 *v*/*v*) solution over a period of one week.

Crystal data

$C_{16}H_{15}N_3O_2$
M_r = 281.31
Monoclinic, $P2_1/c$
a = 8.6112 (9) Å
b = 21.669 (2) Å
c = 8.1152 (8) Å
β = 106.820 (2)°
V = 1449.5 (3) Å^3
Z = 4
D_x = 1.289 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3374 reflections
θ = 2.5–25.9°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.47 × 0.28 × 0.26 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.978
8048 measured reflections
2858 independent reflections
2304 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 26.0°
$h = -10 \rightarrow 10$
$k = -26 \rightarrow 26$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.05
2858 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.2149P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C9	1.2148 (17)	N1—C5	1.372 (2)
O2—C13	1.3613 (17)	N2—N3	1.3511 (17)
O2—C16	1.4271 (18)	N3—C6	1.3555 (19)
N1—N2	1.301 (2)	N3—C7	1.4535 (19)
C13—O2—C16	117.31 (11)	O1—C9—C8	119.20 (14)
O1—C9—C10	121.80 (13)	C10—C9—C8	119.01 (12)

All H atoms were located in a difference Fourier map 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) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms.

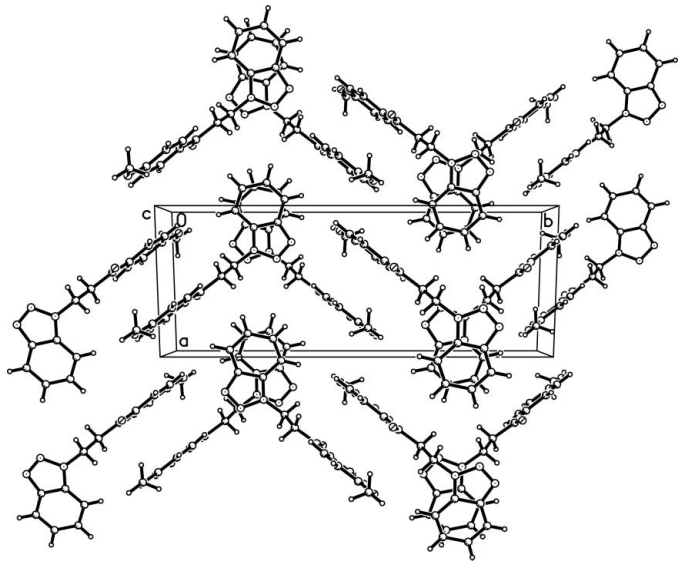


Figure 2
The crystal packing, viewed down the *c* axis.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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