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2-(1*H*-1,2,3-Benzotriazol-1-ylmethyl)-1-(4-methylbenzoyl)ethyl benzoate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.120
Data-to-parameter ratio = 10.7

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

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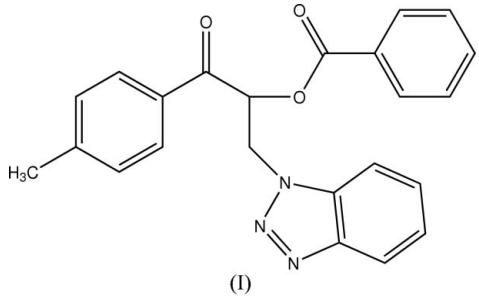
In the title compound, $C_{23}H_{19}N_3O_2$, the molecules are linked into centrosymmetric dimers by C—H···O hydrogen bonds. The packing is further stabilized by C—H···π and π–π interactions.

Comment

In order to search for new benzotriazole compounds with higher bioactivity, the title compound, (I), was synthesized and its structure is presented here. The bond lengths in the benzotriazole ring system show a character intermediate between single and double bonds. The benzotriazole system is almost planar, with a dihedral angle of 0.8 (1)° between the triazole (*A*, atoms N1–N3/C10/C11) and benzene rings (*B*, C10–C15). The dihedral angles between the mean planes of the benzotriazole system and rings *C* (C1–C6) and *D* (C17–C22) are 11.7 (1) and 84.2 (1)°, respectively. The dihedral angle between rings *C* and *D* is 83.7 (1)°. The relative orientation of the three rings is determined by the sp^3-hybridization character of the chiral atom C8.



(I)

In the crystal structure, the molecules are linked into centrosymmetric dimers by weak C—H···O hydrogen bonds (Fig. 2, Table 1). Further weak C—H···O hydrogen bonds connect the dimers into a three-dimensional framework. The packing is also stabilized by C—H···π and π–π interactions involving the benzotriazole ring system, with *Cg*···*Cg* (1 − *x*, 1 − *y*, −*z*) = 3.864 Å, where *Cg* is the centroid of the C10–C15 ring.

Experimental

Bromine (3.2 g, 0.02 mol) was added dropwise to a solution of 3-benzotriazol-1-yl-1-(4-methylphenyl)propan-1-one (5.3 g, 0.02 mol) and sodium acetate (1.6 g, 0.02 mol) in acetic acid (50 ml). The reaction was maintained for 13 h. Water (50 ml) and chloroform (20 ml) were then added. The organic layer was washed successively with a saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate, and the chloroform solution filtered.

The mixture was cooled with ice–water, then an acetone solution (10 ml) of 2-benzoic acid (2.4 g, 0.02 mol) and triethylamine (2.8 ml) was added. The mixture was stirred at room temperature for about 2 h. The solution was then filtered and concentrated. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature over a period of one week.

Crystal data

$C_{23}H_{19}N_3O_3$
M_r = 385.41
Triclinic, $P\overline{1}$
a = 9.5987 (9) Å
b = 10.2272 (9) Å
c = 11.4321 (10) Å
α = 116.482 (1)°
β = 96.928 (1)°
γ = 97.444 (1)°
V = 975.72 (15) Å^3
Z = 2
D_x = 1.312 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.41 × 0.25 × 0.18 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} = 0.984
4423 measured reflections
2808 independent reflections
2400 reflections with $I > 2\sigma(I)$
R_{int} = 0.011
θ_{max} = 23.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.120
S = 1.06
2808 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.235P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23C···Cg^{i}	0.96	2.85	3.572	133
C9—H9A···O1^{ii}	0.97	2.59	3.517 (2)	161
C15—H15A···O1^{ii}	0.93	2.46	3.351 (3)	161

Symmetry codes: (i) $x, y-1, z-1$; (ii) $-x+1, -y, -z$.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl 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).

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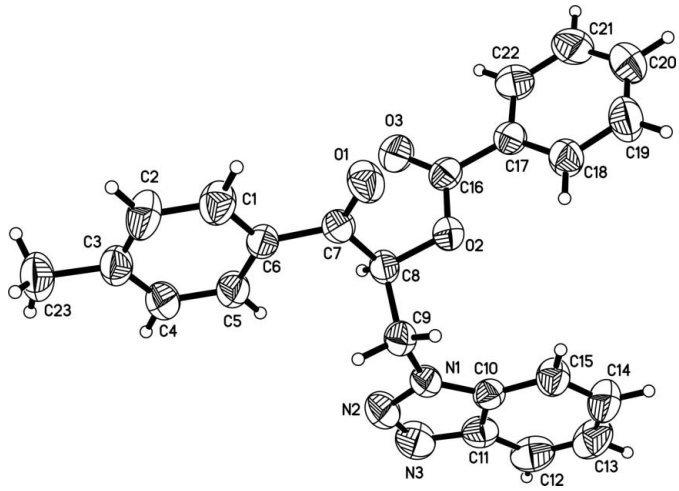

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

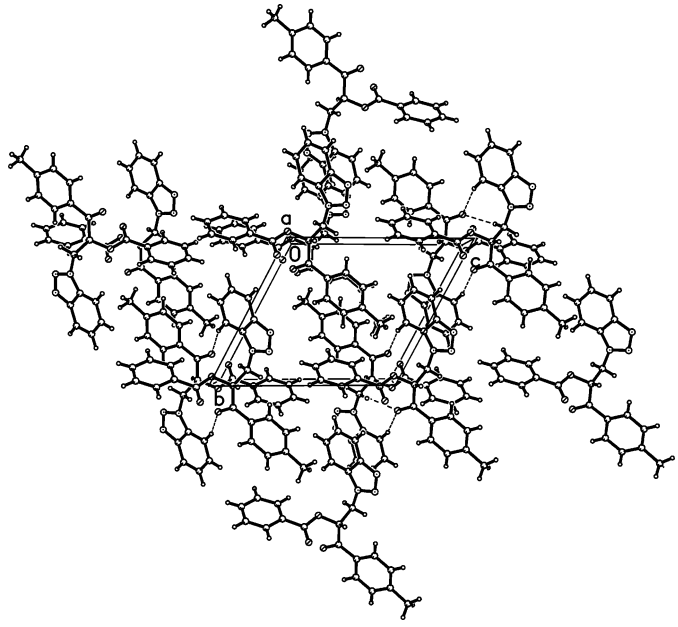

Figure 2
Packing diagram of (I), down the *a* axis, showing the hydrogen-bonded (dashed lines) dimers.

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