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2,6-Di-*tert*-butyl-4-{[2-(1-methyl-1*H*-benzimidazol-2-yl)phenyl]imino}cyclohexa-2,5-dien-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 = 0.044
wR factor = 0.125
Data-to-parameter ratio = 14.3

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

In the title compound, $C_{28}H_{31}N_3O$, the benzimidazole group is close to perpendicular to the benzene ring. Molecules form pairs *via* π–π stacking interactions between benzimidazole groups.

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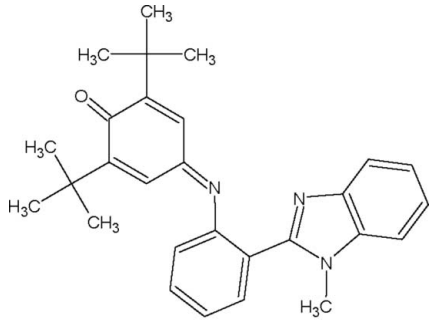
Comment

Benzimidazole derivatives have potential pharmaceutical applications with a broad spectrum of pharmacological actions (Geary *et al.*, 1999; Lage *et al.*, 2006).



(I)

In the title compound, (I) (Fig. 1), all bond lengths and angles are close to standard values (Allen *et al.*, 1987). The benzimidazole fragment lies virtually perpendicular to the C7–C12 benzene ring, with the torsion angle C7—C12—C13—N2 = 82.9 (2)°. The interplanar angle between the C7–C12 benzene and C1–C6 cyclohexadiene rings is 52.0 (1)°. Molecules form pairs via π–π stacking interactions between benzimidazole groups related by a centre of inversion (symmetry code: 1 − *x*, 1 − *y*, 1 − *z*) (Fig. 2). The interplanar distance is 3.37 (1) Å and the centroids of the benzene rings (C14–C19) are offset by 2.61 (1) Å parallel to the ring planes. C—H···O and C—H···N interactions are also present between molecules (Table 1).

Experimental

Crystals of (I) were grown by slow evaporation of a solution in acetonitrile.

Crystal data

$C_{28}H_{31}N_3O$
M_r = 425.56
Triclinic, $P\overline{1}$
a = 10.691 (5) Å
b = 11.963 (5) Å
c = 12.096 (6) Å
α = 96.21 (3)°
β = 115.51 (3)°
γ = 113.25 (3)°
V = 1208.4 (11) Å^3
Z = 2
Mo *Kα* radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.50 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
4487 measured reflections
4242 independent reflections
2876 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
2 standard reflections
every 98 reflections
intensity decay: 3.7%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.125$
$S = 1.01$
4242 reflections
296 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C28—H28B···O1^{i}	0.96	2.76	3.590 (3)	145
C17—H17···N1^{ii}	0.93	2.96	3.851 (3)	161
C26—H26B···N2^{iii}	0.96	2.90	3.805 (3)	157

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

H atoms were placed at calculated positions, with methyl C—H = 0.96 Å and aromatic C—H = 0.93 Å, and refined using a riding model, with U_{iso}(H) = 1.5U_{eq}(methyl C) or 1.5U_{eq}(aromatic C). The methyl groups were allowed to rotate about their local threefold axes.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; 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*.

The CAD-4 diffractometer and software were accessed *via* the X-ray Structural Centre at Moscow, Russia. The author thanks Dr Olekhnovich (Rostov State University, Russia) for providing crystals of (I).

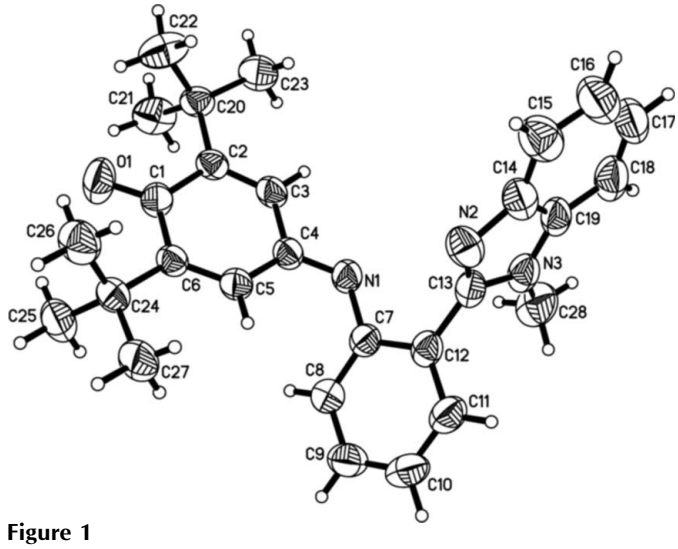


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level for non-H atoms.

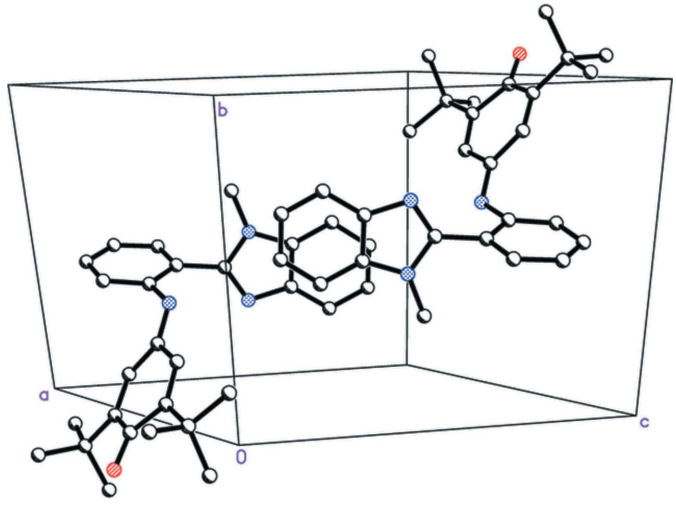


Figure 2
Perspective view of part of the crystal structure of (I), showing a pair of molecules linked by a π–π stacking interaction. H atoms have been omitted.

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