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2,6-Di-*tert*-butyl-4-[(1-methyl-1*H*-benzimidazol-2-yl)-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) = 0.006 Å
R factor = 0.064
wR factor = 0.214
Data-to-parameter ratio = 12.9

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

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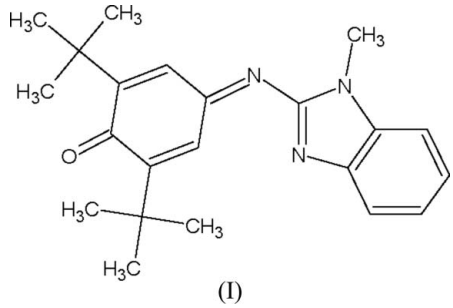
Except for two pairs of methyl groups, all non-H atoms of the title compound, $C_{22}H_{27}N_3O$, occupy special positions on a mirror plane. The molecules are packed in a herring-bone manner and form stacks along [010].

Comment

Compounds containing a benzimidazole group have potential pharmaceutical applications. Some of them exhibit a broad spectrum of pharmacological actions, ranging from anthelmintic activity (Geary *et al.*, 1999) to anticancer therapy (Lage *et al.*, 2006).



(I)

In the title compound, (I), all non-H atoms, except for C16 and C19, together with their symmetry-equivalents, occupy special positions on a mirror plane (Fig. 1). All bond lengths and angles are close to standard values (Allen *et al.*, 1987). Molecules of (I) are packed in stacks extending along [010], within which adjacent molecules are related by inversion operations (symmetry codes: $-x$, $-y$, $1-z$ and $-x$, $1-y$, $1-z$). The interplanar distance within the stacks is 3.39 (1) Å. The stacks are arranged in a herring-bone manner (Fig. 2), with no significant C—H···O or C—H···N interactions between them.

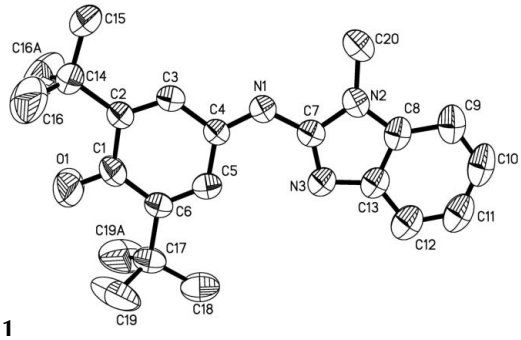


Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. Atoms C16*A* and C19*A* are generated by the symmetry operation $(x, \frac{1}{2}-y, z)$. H atoms have been omitted.

Experimental

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

Crystal data

$C_{22}H_{27}N_3O$
M_r = 349.47
Orthorhombic, *Pnma*
a = 18.372 (4) Å
b = 6.7816 (14) Å
c = 16.833 (3) Å
V = 2097.3 (7) Å^3
Z = 4
D_x = 1.107 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
Prism, yellow
0.50 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1985 measured reflections
1985 independent reflections
996 reflections with $I > 2\sigma(I)$
θ_{max} = 25.0°
2 standard reflections
every 98 reflections
intensity decay: 3.7%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.214
S = 1.00
1985 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1333P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.019 (4)

All H atoms were placed in calculated positions, with C—H = 0.93 (CH) or 0.96 Å (CH_3), and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) (CH) or 1.5U_{eq}(C) (methyl). 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: *SHELXL97*.

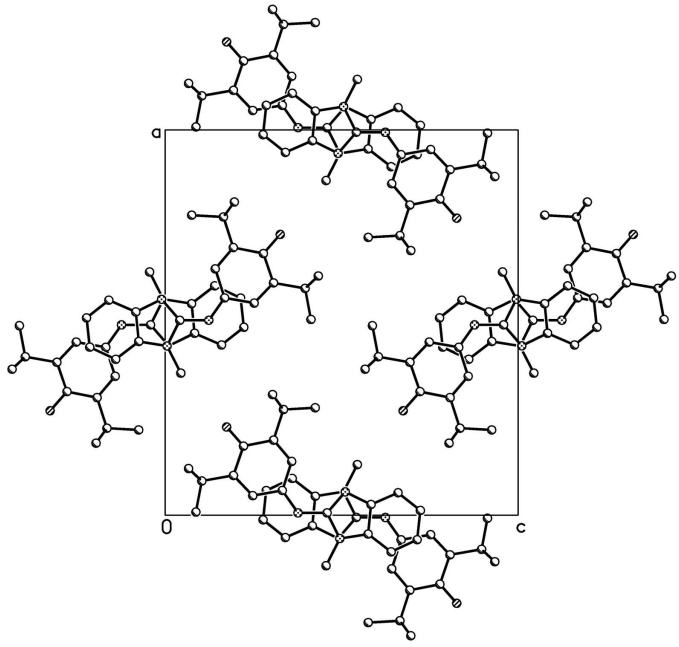


Figure 2
Projection of the crystal structure of (I) along the *b* axis. H atoms have been omitted.

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

References

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