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1-(5,6-Dimethyl-1,2,4-triazin-3-yl)-2-methyl-1*H*-benzimidazole

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Key indicators

Single-crystal X-ray study
T = 243 K
Mean σ(C–C) = 0.002 Å
R factor = 0.058
wR factor = 0.173
Data-to-parameter ratio = 20.8

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

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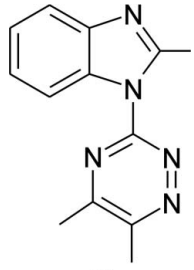
In the title molecule, $C_{13}H_{13}N_5$, all bond lengths and angles show normal values. The molecular skeleton is almost planar; the mean planes of the benzimidazole and triazine rings make a dihedral angle of 1.28 (6)°. The crystal packing is stabilized by π–π interactions and weak intermolecular C—H···N hydrogen bonds.

Comment

In the search for correlation between the structure and reactivity of *N*-cyanoazole derivatives (Pan'kov *et al.*, 2001*a*,*b*), 2-methyl-1*H*-benzimidazole-1-carbohydrazonamide has been synthesized by the reaction of 2-methyl-1-cyanobenzimidazole with hydrazine (Pan'kov *et al.*, 2001*a*). The title compound, (I) (Fig. 1), has been prepared by the reaction of 2-methyl-1*H*-benzimidazole-1-carbohydrazonamide with diacetyl.



(I)

The bond lengths and angles in (I) are normal (Allen *et al.*, 1987). The triazine ring is almost planar, with an r.m.s. deviation of 0.014 (1) Å. The geometry of the triazine ring and the C—N distances indicate a donation of the N5 lone pair into the triazine π system. Furthermore, the benzimidazole and triazine rings in (I) are almost coplanar; the dihedral angle of 1.28 (6)° between the two least-squares planes suggests conjugation between the benzimidazole and triazine ring systems.

In the crystal structure, weak intermolecular C—H···N hydrogen bonds (Table 1) link the molecules into zigzag chains. Two adjacent molecules are paired *via* a π–π interaction, with a short distance of 3.533 (3) Å between the centroid of the triazine ring of one molecule and the centroid of the five-membered ring of another molecule. Both these interactions stabilize the crystal packing (Fig. 2).

Experimental

2-Methyl-1*H*-benzimidazole-1-carbohydrazonamide was prepared according to the procedure of Pan'kov *et al.* (2001*a*). 2-Methyl-1*H*-benzimidazole-1-carbohydrazonamide (5.7 mmol) and diacetyl

(0.5 ml) were dissolved in propan-2-ol (10 ml). The mixture was boiled for 5–6 h and then concentrated to dryness. The solid was recrystallized from ethyl acetate (yield 95%; m.p. 420–421 K).

Crystal data

$C_{13}H_{13}N_5$
M_r = 239.28
Monoclinic, $P2_1/n$
a = 7.412 (4) Å
b = 13.163 (7) Å
c = 12.499 (7) Å
β = 97.701 (11)°
V = 1208.4 (11) Å^3
Z = 4
D_x = 1.315 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 243 (2) K
Prism, colourless
0.60 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.951, T_{max} = 0.983
9157 measured reflections
3459 independent reflections
2213 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 30.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.173
S = 1.07
3459 reflections
166 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0999P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H1···N3^{i}	0.93	2.60	3.423 (2)	148

Symmetry code: (i) $x-\frac{1}{2}, -y-\frac{1}{2}, z-\frac{1}{2}$.

All H atoms were located in a difference map and refined as riding, with C—H = 0.98 (CH_3) or 0.93 Å (CH), and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; 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*.

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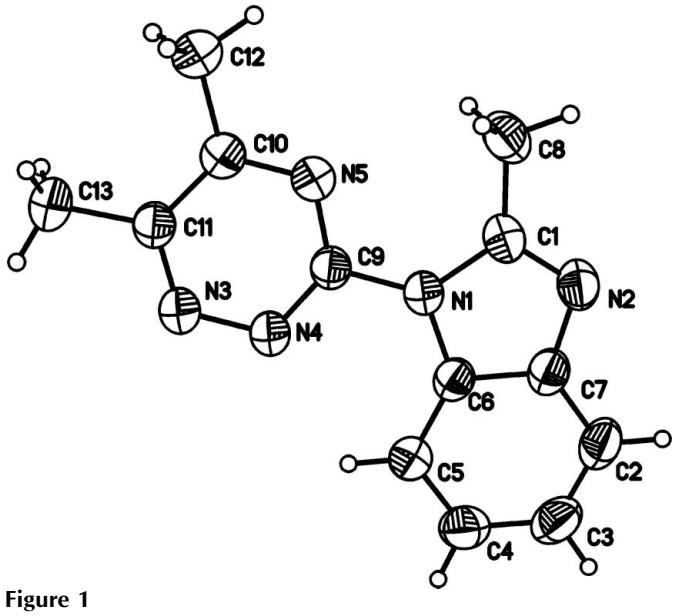

Figure 1
The molecular structure of (I), with the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level.

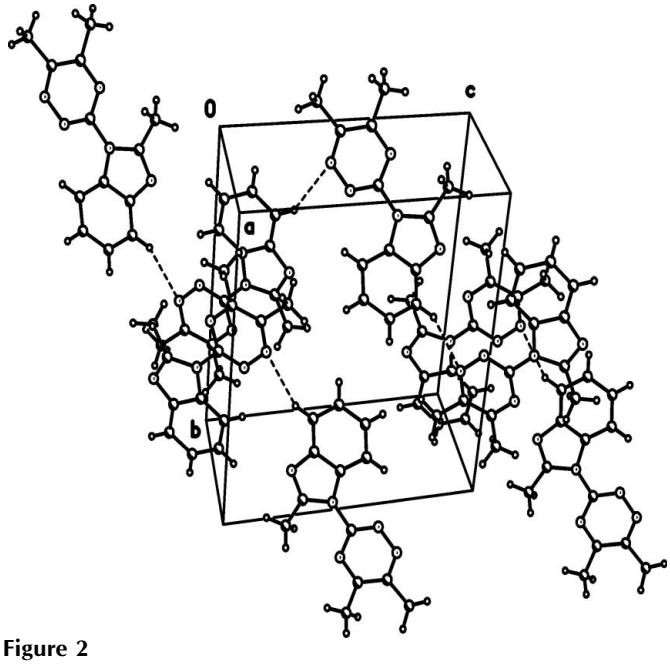

Figure 2
The crystal packing in (I). Hydrogen bonds are shown as dashed lines.

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