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2′-(4-Methylbenzylidene)-5-phenyl-1*H*-pyrazole-3-carbohydrazide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.165
Data-to-parameter ratio = 14.5

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

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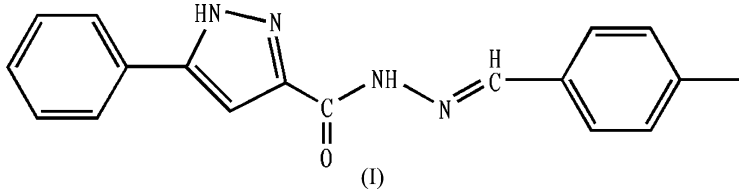
The title compound, $C_{18}H_{16}N_4O$, was prepared by the reaction of 5-phenyl-1*H*-pyrazole-3-carbohydrazide with 4-methylbenzaldehyde in refluxing ethanol. The structure exhibits weak intermolecular N—H···O and N—H···N hydrogen-bonding interactions.

Comment

Schiff bases have been used extensively as ligands in the field of coordination chemistry (Öğretir *et al.*, 2006). As dinegatively charged ligands, Schiff bases show potential as antimicrobial and anticancer agents (Tarafder *et al.*, 2000; Deschamps *et al.*, 2003) and so have biochemical and pharmacological applications. In addition, the chemical behavior of metal complexes with Schiff base ligands has attracted much attention because of their catalytic activity in some industrial and biochemical processes (Wu *et al.*, 2006). The title compound, (I), was synthesized as part of our study of these ligands and we report here the crystal structure of (I).



(I)

In (I) (Fig. 1), the bond lengths and angles in 1*H*-pyrazole are in good agreement with those reported previously (Yang *et al.*, 2003). The C═N and C═O bond lengths are comparable with those reported previously (Ali *et al.*, 2005). Atoms N1, N2, C7, C8, C9 and C6 lie in a plane (*p*5), with a maximum deviation of 0.0093 (3) Å for C7. Phenyl ring C1–C6 and atom C7 are coplanar (*p*7), with a maximum deviation of 0.0088 (3) Å for C7. Benzene ring C12–C17 is approximately coplanar with N4 and C18 (*p*9), with a maximum deviation of 0.0583 (3) Å for N4. The dihedral angles made by *p*5 with *p*7 and *p*9 are 23.12 (1) and 36.16 (1)°, respectively. The dihedral angle between *p*7 and *p*9 is 58.99 (1)°. There are some weak intermolecular N—H···O and N—H···N hydrogen bonding interactions (Table 2), which stabilize the structure of (I).

Experimental

A mixture of 5-phenyl-1*H*-pyrazole-3-carbohydrazide (0.01 mol) with 4-methylbenzaldehyde (0.01 mol) was stirred in refluxing ethanol (30 ml) for 5 h to afford the title compound, (I) (yield: 2.77 g, 81%). Single crystals suitable for X-ray measurements were obtained by recrystallization from dimethylformamide (DMF) at 309 K.

Crystal data

$C_{18}H_{16}N_4O$
M_r = 304.35
Monoclinic, $C2/c$
a = 18.280 (4) Å
b = 14.790 (3) Å
c = 13.364 (3) Å
β = 106.27 (3)°
V = 3468.4 (14) Å^3
Z = 8
D_x = 1.166 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colorless
0.18 × 0.17 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
6290 measured reflections
3053 independent reflections
1730 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.0°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.165
S = 1.02
3053 reflections
210 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0905P)^2 + 0.2393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0061 (8)

Table 1
Selected geometric parameters (Å, °).

O1—C10	1.239 (2)	N4—C11	1.269 (3)
N1—N2	1.343 (2)	C6—C7	1.462 (3)
N1—N2—C9	104.44 (17)	C11—N4—N3	115.60 (19)
C10—N3—H3*A*	120.4	O1—C10—N3	123.8 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.86	2.10	2.813 (2)	140
N3—H3*A*···N2^{ii}	0.86	2.19	2.996 (3)	156

Symmetry codes: (i) $x, -y, z-\frac{1}{2}$; (ii) $-x, y, -z+\frac{3}{2}$.

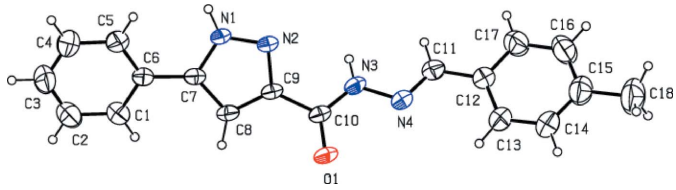


Figure 1
The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H = 0.86 Å and C—H = 0.93–0.96 Å, and with U_{iso}(H) = 1.2–1.5U_{eq} of the parent atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *PARST* (Nardelli, 1996) and *WinGX* (Farrugia, 1999).

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