4-[(Z)-(Benzylamino)phenylmethylene]-5-methyl-2-phenyl-2H-pyrazol-3-one

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Key indicators

Single-crystal X-ray study

T = 293 K

Mean σ(C–C) = 0.003 Å

R factor = 0.043

wR factor = 0.134

Data-to-parameter ratio = 16.5

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

The NH unit on the exocyclic carbon-carbon double bond in the title compound, $C_{24}H_{21}N_3O$, lies on the same side of the double bond as the carbonyl unit of the pyrazolonyl ring, and the two interact through an $N-H \cdots O$ hydrogen bond [2.714 (2) Å].

Comment

This is a study on a compound that is related to 5-methyl-2-phenyl-4-[(Z)-(2-tolylamino)phenylmethylene]-2H-pyrazol-3-one (Bao et al., 2004), one of a class of pyrazolones that are readily synthesized by condensing 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone with a primary amine. The present compound (Fig. 1) has the isomeric benzylimino unit in place of the 2-tolylimino unit. No significant differences are found in the principal bond dimensions for the two compounds; the packing is similar, as noted from their calculated densities. The present compound also features an intramolecular hydrogen bond.

(I)
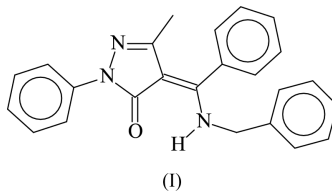
Experimental

1-Phenyl-3-methyl-4-benzoyl-5-pyrazolone (2.5 g, 9 mmol) and benzylamine (1 g, 9 mmol) were dissolved in ethanol (25 ml); the solution was heated under reflux for several hours. The solvent was removed and the pure product obtained upon recrystallization from ethanol in 75% yield.

Crystal data

$C_{24}H_{21}N_3O$	D_x = 1.264 Mg m^{-3}
M_r = 367.44	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 872
a = 8.912 (1) Å	reflections
b = 20.769 (3) Å	θ = 2.5–25.9°
c = 10.608 (1) Å	μ = 0.08 mm^{-1}
β = 79.605 (2)°	T = 293 (2) K
V = 1931.2 (4) Å^3	Prism, yellow
Z = 4	0.50 × 0.38 × 0.14 mm

Data collection

Bruker SMART area-detector diffractometer	2456 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.032
Absorption correction: none	θ_{max} = 27.2°
11972 measured reflections	$h = -11 \rightarrow 11$
4250 independent reflections	$k = -26 \rightarrow 23$
	$l = -10 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.044$	$+ 0.2452P]$
$wR(F^2) = 0.135$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} = 0.001$
4250 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
258 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.247 (2)	C9—C10	1.489 (3)
N1—C7	1.379 (2)	C11—C12	1.478 (2)
N1—N2	1.399 (2)	C18—C19	1.508 (2)
N1—C1	1.412 (2)	C19—C24	1.378 (2)
N2—C9	1.306 (2)	C19—C20	1.386 (2)
N3—C11	1.321 (2)	C20—C21	1.377 (2)
N3—C18	1.450 (2)	C21—C22	1.364 (3)
C7—C8	1.434 (3)	C22—C23	1.369 (3)
C8—C11	1.395 (2)	C23—C24	1.382 (2)
C8—C9	1.428 (2)		
C7—N1—N2	111.6 (1)	C9—C8—C7	105.4 (1)
C7—N1—C1	128.5 (2)	N2—C9—C8	111.7 (2)
N2—N1—C1	119.5 (1)	N2—C9—C10	118.9 (2)
C9—N2—N1	106.5 (1)	C8—C9—C10	129.4 (2)
C11—N3—C18	127.6 (2)	N3—C11—C8	119.2 (2)
C6—C1—N1	121.0 (2)	N3—C11—C12	118.2 (2)
C2—C1—N1	119.3 (2)	C8—C11—C12	122.6 (2)
O1—C7—N1	126.0 (2)	C13—C12—C11	121.3 (2)
O1—C7—C8	129.2 (2)	C17—C12—C11	119.1 (2)
N1—C7—C8	104.9 (2)	N3—C18—C19	114.4 (1)
C11—C8—C9	132.5 (2)	C24—C19—C18	123.5 (2)
C11—C8—C7	122.1 (2)	C20—C19—C18	117.7 (2)

H atoms were placed at calculated positions in the riding model approximation (C—H 0.93 Å for the aromatic H atoms, C—H 0.96 Å for the methyl H atoms and C—H 0.97 Å for the methylene H atoms), with $U_{iso} = 1.2U_{eq}$(parent atom) for the aromatic and methyl C atoms, and $1.5U_{eq}$ for the methyl C atom. The amino H atom was located and refined.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve
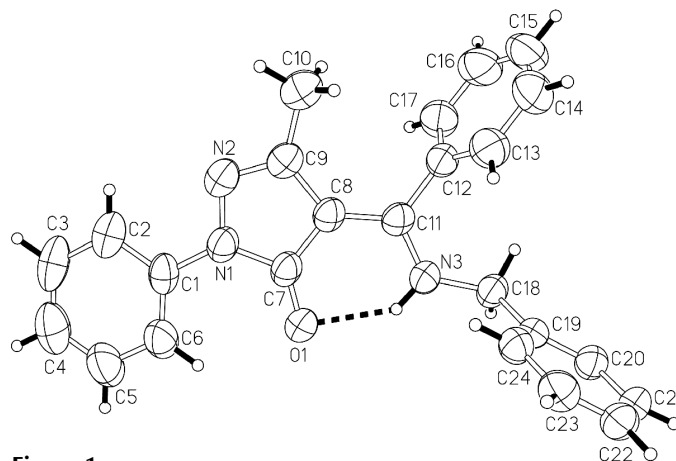

Figure 1
*ORTEP*II (Johnson, 1976) plot of $C_{24}H_{21}N_3O$, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*I;I (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

References

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