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1-Benzyl-2-[1-(5-methyl-1*H*-pyrazol-3-yl)-2-phenylethyl]benzimidazole

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.130
Data-to-parameter ratio = 18.0

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

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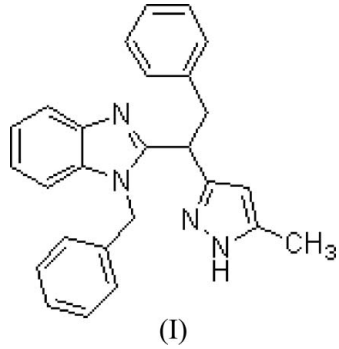
The title compound, $C_{26}H_{24}N_4$, contains one pyrazole ring and two phenyl rings, which are nearly perpendicular to the benzimidazole ring system. In the structure, there is one intramolecular C—H···N hydrogen-bonding interaction.

Comment

Benzimidazole derivatives are compounds that have received much attention because of their applications in several areas. They are used as antibacterial (Özden *et al.*, 2004), anticancer (Easmon *et al.*, 2001; Zhu *et al.*, 1999), anti-inflammatory (Tewari & Mishra, 2001) and antiulcer agents (Shafik *et al.*, 2004; El-Naem *et al.*, 2003). They also have herbicidal, insecticidal and complexing properties (Sbai *et al.*, 2003, 2002; Attar *et al.*, 2001).



(I)

An *ORTEP-3* (Farrugia, 1997) drawing of (I) is shown in Fig. 1. All geometric parameters of (I) are normal and are consistent with those in similar compounds (Allen *et al.*, 1987). The dihedral angle between the two phenyl rings [ring *A* (atoms C14–C19) and ring *B* (atoms C21–C26)] is 61.85 (12)°. The pyrazole ring is nearly perpencicular to the benzimidazole ring system; the dihedral angle between the pyrazole and benzimidazole planes is 77.25 (8)°.

The crystal structure has one intramolecular C–H···N hydrogen bonding interaction. There are no classical hydrogen bonds in the structure.

Experimental

Hydrazine hydrate (0.29 cc, 0.006 mol) was added to a solution of (4*Z*)-(2-oxopropylidene)-1,3-dibenzyl-1,2,4,5-tetrahydro-2*H*-1,5-benzodiazepin-2-one (1.17 g, 0.003 mol) in ethanol (30 ml). The reaction mixture was heated at reflux for 8 h; after cooling, a solid was isolated and dried under vacuum (yield 82%). ^{1}H NMR ($CDCl_3$, p.p.m.): δ 2.34 (*s*, 3H, CH_3), 3.75 (*dd*, 2H, CH_2, ^2J = 6.9 Hz), 4.76 (*t*, 1H, CH), 5.42 (*dd*, 2H, NCH_2, ^2J = 17.1 Hz), 6.11 (*s*, 1H, CH), 6.91–8.01 (CH_{Ar}). ^{13}C NMR ($CDCl_3$, p.p.m.) δ: 11.8, 40.8, 47.1, 103.2, 109.8,

119.4, 122.1, 122.5, 126.1, 126.3, 127.5, 128.2, 128.7, 129.1, 135.2, 135.6, 135.9, 139.3, 142.5, 155.1.

Crystal data

$C_{26}H_{24}N_4$	$Z = 2$
$M_r = 392.49$	$D_x = 1.219$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.244$ (5) Å	Cell parameters from 21742 reflections
$b = 10.601$ (5) Å	$\theta = 2.2$–$27.9°$
$c = 11.404$ (5) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 64.499$ (5)°	$T = 296$ K
$\beta = 74.587$ (5)°	Prism, colourless
$\gamma = 89.556$ (5)°	0.62 × 0.53 × 0.47 mm
$V = 1069.5$ (9) Å^3	

Data collection

Stoe IPDS-II diffractometer	$R_{int} = 0.120$
ω scans	$\theta_{max} = 27.8°$
Absorption correction: none	$h = -13 \rightarrow 13$
17823 measured reflections	$k = -13 \rightarrow 13$
4925 independent reflections	$l = -14 \rightarrow 14$
3537 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 0.0775P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.046$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.130$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.32$ e Å^{-3}
4925 reflections	Extinction correction: *SHELXL97*
273 parameters	Extinction coefficient: 0.020 (5)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C6	1.385 (2)	N2—C20	1.4543 (19)
N1—C7	1.307 (2)	N3—N4	1.401 (2)
N2—C1	1.383 (2)	N3—C9	1.302 (2)
N2—C7	1.3710 (19)	N4—C11	1.333 (2)
C6—N1—C7	104.67 (12)	N1—C6—C5	129.79 (14)
C1—N2—C7	105.93 (11)	N2—C7—C8	122.51 (12)
C1—N2—C20	125.09 (12)	N1—C7—C8	123.69 (13)
C7—N2—C20	128.96 (13)	N1—C7—N2	113.63 (14)
N4—N3—C9	105.52 (13)	N3—C9—C8	119.42 (14)
N3—N4—C11	108.75 (13)	N3—C9—C10	111.30 (14)
N2—C1—C2	131.71 (14)	N4—C11—C12	117.71 (17)
N2—C1—C6	105.50 (13)	N4—C11—C10	109.55 (16)
N1—C6—C1	110.28 (14)	N2—C20—C21	115.01 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
C26—H26···N2	0.93	2.58	2.900 (3)	101

All H atoms were positioned geometrically and refined using a riding model [U_{iso}(H) = 1.5U_{eq}(C) for methyl groups and 1.2U_{eq}(C,N) for other atoms; N—H = 0.86 Å; C—$H_{aromatic}$ = 0.93 Å, methyl C—H = 0.96 Å, methylene C—H = 0.97 Å and C8—H8 = 0.98 Å]. The methyl group was allowed to rotate but not to tip.

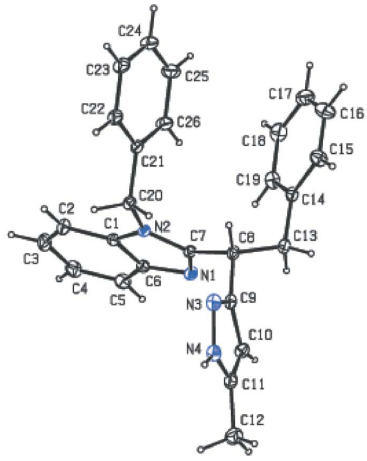


Figure 1
A view of (I), with the atom-numbering scheme and 10% probability displacement ellipsoids.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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