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3-Methyl-1-phenyl-*N*-(2-thienylmethylene)-1*H*-pyrazol-5-amine

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.131
Data-to-parameter ratio = 14.0

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

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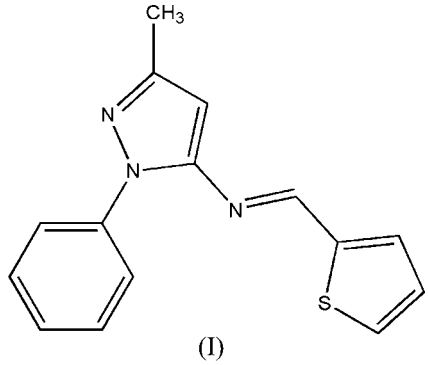
The title compound, $C_{15}H_{13}N_3S$, was synthesized by the reaction of 3-methyl-1-phenyl-1*H*-pyrazol-5-amine and thiophene-2-carbaldehyde in boiling ethanol. The dihedral angle between the thiophene and pyrazole planes is 14.7 (1)° and the phenyl ring is twisted from the attached pyrazole ring by 32.2 (1)°.

Comment

Schiff bases are considered as a very important class of organic compounds which have wide applications in many biological situations (Fridovitch & Westheimer, 1962). The reaction of 2-carbaldehyde and 2,6-dicarbaldehyde derivatives with a diamine results in open-chain and macrocyclic Schiff bases, respectively (Janusz *et al.*, 2004). Studies performed on the synthesis and complexation behaviour of macrocyclic Schiff bases derived from 2,6-thiophene dicarbaldehyde are considerably more numerous compared with those of open-chain Schiff bases derived from 2-thiophene carbaldehyde (Hashemia *et al.*, 2001). Studies on the synthesis and metal chelating properties of 2-thiophene carbaldehyde derivatives are very limited (Coakley *et al.*, 1969; Eichhorn & Bailar, 1953). We report here the crystal structure of the title compound, (I).



(I)

In the title molecule (Fig. 1), the dihedral angle between the thiophene (S1/C5–C8) and pyrazole (N1/N2/C1–C3) planes is 14.7 (1)°. The C9–C14 phenyl ring is twisted from the attached pyrazole ring by 32.2 (1)°. An intramolecular C14—H14···N3 hydrogen bond [H14···N3 = 2.47 Å, C14—N3 = 2.965 (4) Å and C14—H14···N3 = 114°] is observed.

Experimental

Compound (I) was synthesized by the reaction of 3-methyl-1-phenyl-1*H*-pyrazol-5-amine (2 mmol) and thiophene-2-carbaldehyde (2 mmol) in boiling ethanol (10 ml). Single crystals of (I) suitable for

X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{15}H_{13}N_3S$	$Z = 4$
$M_r = 267.34$	$D_x = 1.296$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 10.035$ (4) Å	$\mu = 0.23$ mm^{-1}
$b = 8.194$ (3) Å	$T = 298$ (2) K
$c = 16.671$ (7) Å	Block, yellow
$\beta = 92.438$ (5)°	0.38 × 0.20 × 0.17 mm
$V = 1369.6$ (9) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	6774 measured reflections
	2403 independent reflections
φ and ω scans	1499 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.031$
	$\theta_{max} = 25.0°$
$T_{min} = 0.919$, $T_{max} = 0.963$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.6009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.043$	
$wR(F^2) = 0.131$	
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
2403 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
172 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
H-atom parameters constrained	

All H atoms were positioned geometrically and treated as riding, with C—H = 0.93 or 0.96 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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: *SHELXTL*.

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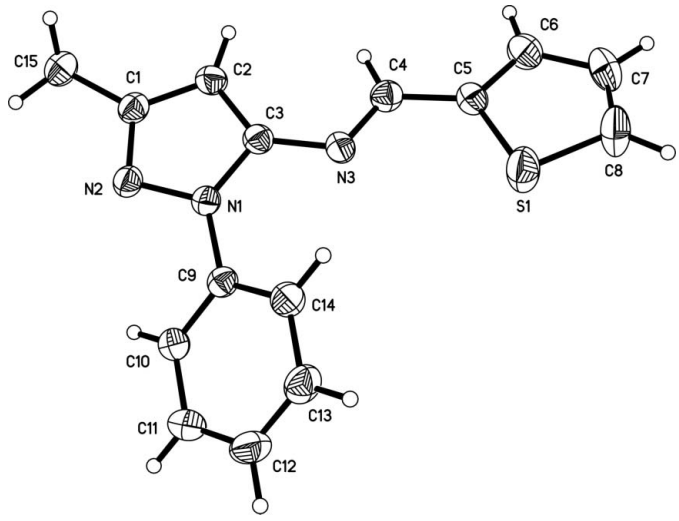

Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

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