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4-{[(*E*)-(3,5-Dimethyl-1-phenyl-1*H*-pyrazol-4-yl)methylidene]amino}-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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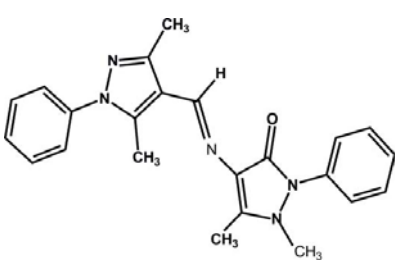
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.059; wR factor = 0.161; data-to-parameter ratio = 19.3.

The title Schiff base compound, $C_{23}H_{23}N_5O$, was synthesized by the reaction of 4-aminophenazone and 3,5-dimethyl-1-phenylpyrazole-4-carbaxaldehyde. The molecule adopts an *E* configuration about the central C=N double bond. A weak intramolecular C—H···O hydrogen bond generates an *S*(6) ring motif. The dihedral angle between the pyrazole rings is 24.72 (10)° and the dihedral angles between the pyrazole rings and the adjacent phenyl rings are 58.67 (10) and 46.58 (11)°. The crystal structure is stabilized by weak C—H···π interactions involving the pyrazolone and phenyl rings.

Related literature

For background to and applications of heterocylic Schiff bases, see: Nawaz *et al.* (2009); Li *et al.* (1999); Urena *et al.* (2003); Geronikaki *et al.* (2003); Shanker *et al.* (2009); Pandeya *et al.* (1999); Sridhar *et al.* (2002); Nawrocka *et al.* (2004). For related structures, see: Eryigit & Kendi (1998); Manikandan *et al.* (2000). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{23}H_{23}N_5O$
M_r = 385.46
Monoclinic, $P2_1/c$
a = 15.2985 (2) Å
b = 7.6827 (1) Å
c = 19.6737 (3) Å
β = 116.905 (1)°
V = 2062.03 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.45 × 0.21 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.965, T_{max} = 0.992
23014 measured reflections
5993 independent reflections
2881 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.161
S = 1.03
5993 reflections
311 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the N4/N5/C11–C13 and C1–C6 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10*A*···O1	0.986 (18)	2.40 (2)	3.052 (3)	123.3 (14)
C19—H19*A*···*Cg*2^{i}	0.990 (19)	2.656 (19)	3.452 (2)	137.4 (17)
C20—H20*C*···*Cg*1^{ii}	0.96	2.85 (3)	3.720 (3)	149 (1)
C22—H22*B*···*Cg*2^{iii}	0.96	2.82 (3)	3.585 (3)	135 (1)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5060).

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