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4-{[4-(Dimethylamino)benzylidene]-amino}-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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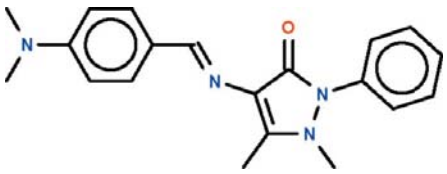
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.101; data-to-parameter ratio = 17.2.

The azomethine double-bond in the title Schiff base, $C_{20}H_{22}N_4O$, has an *E*-configuration. The aromatic ring of the benzylidene portion (r.m.s. deviation 0.011 Å) and the five-membered pyrazolyl ring (r.m.s. deviation 0.033 Å) form a dihedral angle of 19.0 (1)°. The phenyl substituent is twisted by 55.0 (1)° with respect to the five-membered ring.

Related literature

For background to Schiff bases derived from 4-aminoantipyridine, see: Montalvo-González & Ariza-Castolo (2003).



Experimental

Crystal data

$C_{20}H_{22}N_4O$
M_r = 334.42
Monoclinic, $C2/c$
a = 17.7275 (14) Å
b = 6.7552 (6) Å
c = 29.387 (2) Å
β = 101.426 (1)°
V = 3449.5 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
15916 measured reflections
3959 independent reflections
3146 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.101
S = 1.02
3959 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2268).

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