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4-[(9-Ethyl-9*H*-carbazol-3-yl)methylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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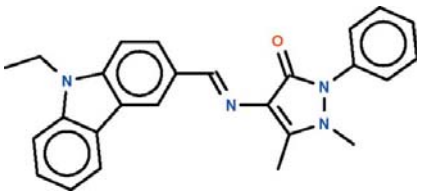
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.104; data-to-parameter ratio = 16.8.

The imino–carbon double bond in the title Schiff base, $C_{26}H_{24}N_4O$, has an E configuration. The 13-membered carbazolyl fused-ring (r.m.s. deviation = 0.056 Å) is nearly coplanar with five-membered pyrazole ring (r.m.s. deviation = 0.036 Å) [dihedral angle between the two systems = 10.4 (1)°]; the phenyl substituent is twisted by 51.1 (1)° with respect to the five-membered ring.

Related literature

For background to this class of Schiff bases, see: Montalvo-González & Ariza-Castolo (2003).



Experimental

Crystal data

$C_{26}H_{24}N_4O$
M_r = 408.49
Monoclinic, $P2_1/n$
a = 10.4458 (6) Å
b = 18.2674 (11) Å
c = 10.8989 (6) Å
β = 96.127 (1)°
V = 2067.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
19772 measured reflections
4756 independent reflections
4000 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.104
S = 1.02
4756 reflections
283 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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: JH2169).

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