

N-[(9-Ethyl-9H-carbazol-3-yl)methylidene]-3,4-dimethylisoxazol-5-amine

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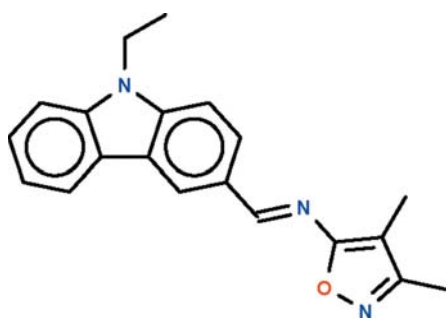
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.089; wR factor = 0.262; data-to-parameter ratio = 12.7.

The azomethine double bond in the title Schiff base, $\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}$, has an *E* configuration. The 13-membered carbazolyl fused ring system [r.m.s. deviation = 0.023 (9) Å] is nearly coplanar with the five-membered pyrazole ring [r.m.s. deviation = 0.003 (4) Å]; the dihedral angle between the two systems is 10.8 (2)°. The crystal studied was a non-merohedral twin having a 35% minor component.

Related literature

For the synthesis and spectroscopic characterization of the title compound, see: Asiri *et al.* (2010). For the treatment of non-merohedral twins, see: Spek (2009).



Experimental

Crystal data

$\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}$
 $M_r = 317.38$
Monoclinic, $P2_1/c$
 $a = 8.0575$ (9) Å
 $b = 13.4483$ (15) Å
 $c = 14.8488$ (16) Å
 $\beta = 94.049$ (2)°

$V = 1605.0$ (3) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 100$ K
0.20 × 0.15 × 0.05 mm

Data collection

Bruker SMART APEX
diffractometer
11993 measured reflections

2811 independent reflections
2286 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.089$
 $wR(F^2) = 0.262$
 $S = 1.11$
2811 reflections

221 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.54$ 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: RK2213).

References

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