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N-[4-(Dimethylamino)benzylidene]-3,4-dimethylisoxazol-5-amine

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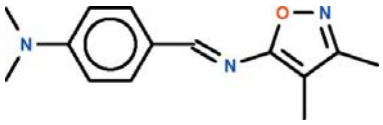
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.113; data-to-parameter ratio = 17.1.

The aromatic rings attached to the azomethine double bond in the title compound, $C_{14}H_{17}N_3O$, are *trans* to each other [C—C═N—C torsion angle = 179.5 (1)°], and they are approximately coplanar [dihedral angle between the five- and six-membered rings = 13.7 (1)°].

Related literature

For the spectroscopic characterization of a related Schiff base, see: Asiri *et al.* (2010).



Experimental

Crystal data

$C_{14}H_{17}N_3O$
M_r = 243.31
Triclinic, $P\overline{1}$
a = 6.5772 (6) Å
b = 9.1246 (9) Å
c = 10.538 (1) Å
α = 92.995 (1)°
β = 95.183 (1)°
γ = 90.873 (1)°
V = 628.86 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.35 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
6092 measured reflections
2866 independent reflections
2401 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.113
S = 1.04
2866 reflections
168 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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: JH2170).

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