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2-[(*E*)-(3,4-Dimethylisoxazol-5-yl)iminomethyl]phenol

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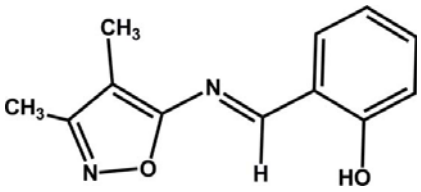
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.070; wR factor = 0.203; data-to-parameter ratio = 16.2.

The title compound, $C_{12}H_{12}N_2O_2$, has been synthesized by the reaction of 5-amino-3,4-dimethylisoxazole and salicyladehyde. The molecule adopts an *E* configuration about the central C=N double bond. The dihedral angle between the isoxazole and phenyl rings is 4.2 (2)° and an intramolecular O—H···N hydrogen bond generates an *S*(6) ring motif. The crystal studied was a non-merohedral twin with a domain ratio of 0.834 (4):0.166 (4).

Related literature

For background to the biological and pharmacological properties of oxazole derivatives, see: Spinelli (1999); Conti *et al.* (1998); Mishra *et al.* (1998); Ko *et al.* (1998); Kang *et al.* (2000); Huang & Chen (2005). For details of hydrogen bonding and hydrogen-bond motifs, see: Jeffrey & Saenger (1991); Bernstein *et al.* (1995); Jeffrey (1997); Scheiner (1997). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{12}H_{12}N_2O_2$
M_r = 216.24
Triclinic, $P\overline{1}$
a = 5.3475 (14) Å
b = 8.615 (2) Å
c = 12.321 (3) Å
α = 103.696 (5)°
β = 91.486 (5)°
γ = 94.059 (5)°
V = 549.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.56 × 0.14 × 0.08 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.951, T_{max} = 0.993
2467 measured reflections
2467 independent reflections
1946 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.203
S = 1.06
2467 reflections
152 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1*O2*···N1	1.00 (9)	1.71 (8)	2.648 (5)	154 (8)

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: SJ2738).

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