Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3,4-Dimethyl-*N*-[(*E*)-3-nitrobenzylidene]-1,2-oxazol-5-amine

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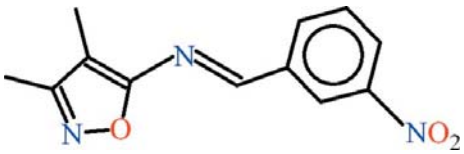
Received 5 September 2010; accepted 6 September 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.061; wR factor = 0.161; data-to-parameter ratio = 12.3.

In the title compound, $C_{12}H_{11}N_3O_3$, the dihedral angle between the 3-nitrobenzaldehyde and 5-amino-3,4-dimethyl-1,2-oxazole moieties is 2.46 (12)°. The molecule is close to planar, the r.m.s. deviation for the non-H atoms being 0.028 Å. The packing only features van der Waals interactions between the molecules.

Related literature

For background and related crystal structures, see: Asiri *et al.* (2010*a*,*b*,*c*,*d*).



Experimental

Crystal data

$C_{12}H_{11}N_3O_3$
M_r = 245.24
Monoclinic, $P2_1/c$
a = 12.602 (2) Å
b = 3.9267 (6) Å
c = 23.366 (4) Å
β = 94.791 (9)°
V = 1152.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.22 × 0.08 × 0.06 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.992, T_{max} = 0.995
8616 measured reflections
2046 independent reflections
846 reflections with $I > 2\sigma(I)$
R_{int} = 0.097

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.161
S = 0.99
2046 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors would like to thank the Chemistry Department, King Abdul Aziz University, Jeddah, Saudi Arabia for providing research facilities and for the financial support of this work *via* grant No. (3–045/430).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5634).

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