Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Chlorobenzylidene)-3,4-dimethylisoxazol-5-amine

Abdullah M. Asiri,[a,b] Salman A. Khan[b] and M. Nawaz Tahir[c]*

[a]The Center of Excellence for Advanced Materials Research, King Abdul Aziz University, Jeddah 21589, PO Box 80203, Saudi Arabia, [b]Department of Chemistry, Faculty of Science, King Abdul Aziz University, Jeddah 21589, PO Box 80203, Saudi Arabia, and [c]Department of Physics, University of Sargodha, Sargodha, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

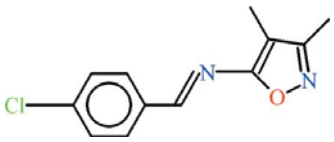
Received 18 July 2010; accepted 22 July 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.120; data-to-parameter ratio = 14.4.

The molecule of the title compound, $C_{12}H_{11}ClN_2O$, has E configuration at the azomethine double bond and is virtually planar with a dihedral angle of 1.25 (13)° between the benzene and isoxazole rings. C—H···π interactions stabilize the crystal structure.

Related literature

For related structures, see: Asiri *et al.* (2010*a*,*b*); Fun *et al.* (2010*a*,*b*); Shad *et al.* (2008); Tahir *et al.* (2008). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{12}H_{11}ClN_2O$
M_r = 234.68
Monoclinic, $P2_1/n$
a = 5.0877 (2) Å
b = 24.5197 (9) Å
c = 9.4673 (4) Å
β = 94.871 (2)°
V = 1176.77 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 296 K
0.30 × 0.16 × 0.14 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.868, T_{max} = 0.965
9016 measured reflections
2112 independent reflections
1539 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
S = 1.07
2112 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

*Cg*1 is the centroid of the O1/N2/C10/C9/C8 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11*C*···*Cg*1^{i}	0.96	2.91	3.644 (2)	134

Symmetry code: (i) $x+1, y, z$.

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 for Windows* (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.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2296).

References

Asiri, A. M., Khan, S. A. & Tahir, M. N. (2010*a*). *Acta Cryst.* E**66**, o2077.
Asiri, A. M., Khan, S. A., Tan, K. W. & Ng, S. W. (2010*b*). *Acta Cryst.* E**66**, o1783.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Fun, H.-K., Hemamalini, M., Asiri, A. M. & Khan, S. A. (2010*a*). *Acta Cryst.* E**66**, o1037–o1038.
Fun, H.-K., Hemamalini, M., Asiri, A. M., Khan, S. A. & Khan, K. A. (2010*b*). *Acta Cryst.* E**66**, o773–o774.
Shad, H. A., Chohan, Z. H., Tahir, M. N. & Khan, I. U. (2008). *Acta Cryst.* E**64**, o635.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tahir, M. N., Chohan, Z. H., Shad, H. A. & Khan, I. U. (2008). *Acta Cryst.* E**64**, o720.