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N-[(*E*)-1,3-Benzodioxol-5-ylmethylidene]-3,4-dimethyl-1,2-oxazol-5-amine

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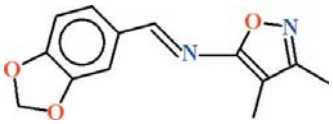
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.132; data-to-parameter ratio = 12.6.

In the title compound, $C_{13}H_{12}N_2O_3$, the dihedral angle between the aromatic rings is 7.94 (12)°. In the crystal, inversion dimers linked by pairs of C—H···O hydrogen bonds generate $R_2^2(6)$ loops. Weak π–π [centroid–centroid separations = 3.7480 (13) and 3.9047 (13) Å] and C—H···π interactions help to consolidate the packing.

Related literature

For background to conjugated azo-methanes, see: Asiri & Khan (2010). For related structures, see: Asiri *et al.* (2010); Tahir *et al.* (2010). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{13}H_{12}N_2O_3$
M_r = 244.25
Monoclinic, $P2_1/n$
a = 7.5759 (5) Å
b = 10.6980 (9) Å
c = 14.6307 (12) Å
β = 102.607 (2)°
V = 1157.19 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.28 × 0.24 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.975, T_{max} = 0.980
8018 measured reflections
2087 independent reflections
1447 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.132
S = 1.03
2087 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7*B*···O1^{i}	0.97	2.58	3.264 (3)	128
C12—H12*A*···*Cg*1^{ii}	0.96	2.95	3.763 (2)	143

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6330).

References

Asiri, A. M. & Khan, S. A. (2010). *Molecules*, **15**, 6850–6858.
Asiri, A. M., Khan, S. A. & Tahir, M. N. (2010). *Acta Cryst.* E**66**, o2127.
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.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tahir, M. N., Shad, H. A., Khan, M. N. & Tariq, R. H. (2010). *Acta Cryst.* E**66**, o3293.