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N-(4-Bromobenzylidene)-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

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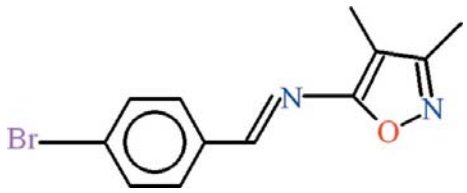
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.025; wR factor = 0.059; data-to-parameter ratio = 14.4.

In the title compound, $C_{12}H_{11}BrN_2O$, the 4-bromobenzaldehyde and 5-amino-3,4-dimethylisoxazole units are oriented at a dihedral angle of 4.89 (8)°. In the crystal, weak π–π interactions are present between the benzene rings at a centroid–centroid distance of 3.7862 (14) Å.

Related literature

For related structures, see: Asiri *et al.* (2010): 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

$C_{12}H_{11}BrN_2O$
M_r = 279.14
Triclinic, $P\overline{1}$
a = 7.6406 (4) Å
b = 8.8709 (5) Å
c = 9.1052 (5) Å
α = 97.024 (2)°
β = 102.961 (1)°
γ = 92.786 (2)°
V = 595.06 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.43 mm^{-1}
T = 296 K
0.30 × 0.14 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.568, T_{max} = 0.665
8212 measured reflections
2119 independent reflections
1643 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.059
S = 1.03
2119 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 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 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: BQ2226).

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