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4-[(7-Fluoroquinazolin-4-yl)oxy]aniline

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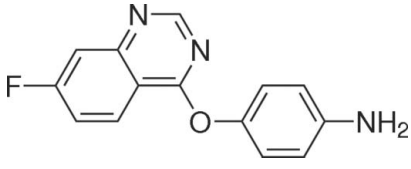
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.110; data-to-parameter ratio = 7.3.

In the molecule of the title compound, $C_{14}H_{10}FN_3O$, the bicyclic quinazoline system is effectively planar, with a mean deviation from planarity of 0.0140 (3) Å. The quinazoline heterocyclic system and the adjacent benzene ring make a dihedral angle of 85.73 (9)°. Two intermolecular N—H···N hydrogen bonds contribute to the stability of the crystal structure. In addition, a weak π–π stacking interaction [centroid–centroid distance = 3.902 (2) Å] is observed.

Related literature

For general background to quinazolines, see: Labuda *et al.* (2009). Graves *et al.* (2002); For the preparation of the title compound, see: Zhang *et al.* (2010). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{10}FN_3O$
M_r = 255.25
Orthorhombic, $P2_12_12_1$
a = 8.0210 (16) Å
b = 8.3370 (17) Å
c = 17.562 (4) Å
V = 1174.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.969, T_{max} = 0.990
2351 measured reflections
1256 independent reflections
883 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.110
S = 1.02
1256 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.89	2.67	3.408 (4)	142
N1—H1B···N3^{ii}	0.89	2.38	3.205 (4)	154

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2317).

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