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N-(2-Fluorobenzylidene)-2,6-diisopropylaniline

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.195
Data-to-parameter ratio = 18.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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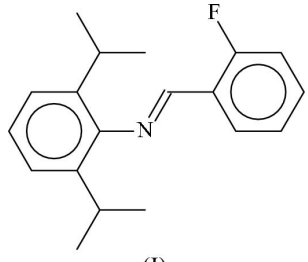
In the molecule of the title Schiff base, $C_{19}H_{22}FN$, the fluorine-bearing aromatic ring makes an angle of 68.0 (1)° with the other sterically crowded aromatic ring.

Comment

A previous structural study of a crowded Schiff base mentions the usefulness of their nickel complexes in catalysis (Gao *et al.*, 2004); steric crowding in the Schiff base appears to be related to catalytic activity. The title compound, (I) (Fig. 1), was designed to have a fluorine substituent in the *ortho* position of the benzene ring to allow it to undergo substitution by alkylamino and arylamino nucleophiles, to form chelating diamines. The two aromatic rings are twisted by 68.0 (1)° relative to each other; both isopropyl substituents are rotated such that the methyl groups point away from the C═N fragment.



(I)

Experimental

A hexane (15 ml) solution of 2-fluorobenzaldehyde (3.28 ml, 3.83 g, 30.9 mmol) and 2,6-diisopropylaniline (6.42 ml, 6.03 g, 34.0 mmol) was stirred for 2 h at room temperature, after which magnesium sulfate was added to ensure complete removal of water. The mixture was filtered and the yellow solution cooled to 263 K to furnish 4.49 g of the yellow Schiff base. Removal of the solvent yielded an additional 1.43 g; yield approximately 70%. Elemental analysis calculated for $C_{19}H_{22}FN$: C 80.53, H 7.83, N 8.94%; found: C 80.37, H 7.54, N 4.73%.

Crystal data

$C_{19}H_{22}FN$
M_r = 283.38
Triclinic, $P\overline{1}$
a = 8.265 (1) Å
b = 10.510 (1) Å
c = 10.841 (1) Å
α = 113.855 (2)°
β = 98.767 (2)°
γ = 98.390 (2)°
V = 828.5 (2) Å^3
Z = 2
D_x = 1.136 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 982 reflections
θ = 2.1–27.1°
μ = 0.07 mm^{-1}
T = 295 (2) K
Block, yellow
0.50 × 0.42 × 0.22 mm

Data collection

Bruker SMART area-detector diffractometer	2421 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.013$
Absorption correction: none	$\theta_{max} = 27.2^\circ$
7091 measured reflections	$h = -10 \rightarrow 10$
3581 independent reflections	$k = -13 \rightarrow 13$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1003P)^2 + 0.1118P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.055$	
$wR(F^2) = 0.195$	
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
3581 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
190 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
H-atom parameters constrained	

H atoms were placed in calculated positions (C—H = 0.93 Å for aromatic H atoms, 0.98 Å for methine H atoms and 0.96 Å for methyl H atoms) and were included in the refinement in the riding-model approximation, with U_{iso}(H) values set at 1.2 times U_{eq} of the parent C atoms, except for the methyl H atoms, for which this was set at 1.5 times U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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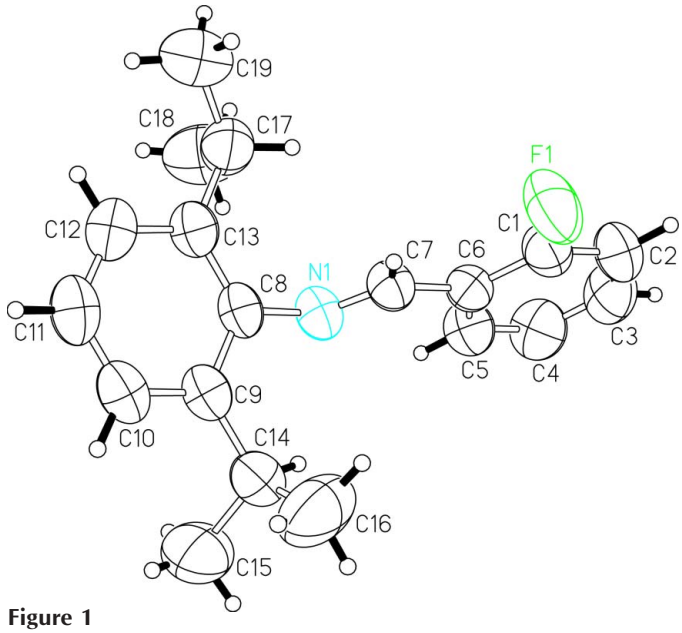

Figure 1
A plot of the molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

References

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