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4-Chloro-2-[(*E*)-(4-fluorophenyl)methyliminomethyl]phenol

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The title compound, $C_{14}H_{11}ClFNO$, forms an intramolecular O—H···N hydrogen bond. The dihedral angle between the two benzene rings is 71.6 (2)°.

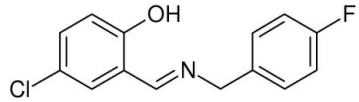
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.058
wR factor = 0.171
Data-to-parameter ratio = 17.6

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

Comment

Salicylaldehyde and its derivatives play an important role in developing molecular architectures in coordination chemistry (Mukhopadhyay *et al.*, 2003; Erxleben & Schumacher, 2001). As Lewis base ligands, the adducts of aldehydes with various primary amines are of interest in a large number of transition-metal complexes (Sreenivasulu *et al.*, 2005; Ranford *et al.*, 1999). Recently, we have reported the structural characterization of two Schiff base compounds derived from the condensation of salicylaldehyde and primary amines (Li *et al.*, 2005, 2006). As an extension of this work, we report here the crystal structure of the title compound, (I).



(I)

In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The C7═N1 bond length of 1.264 (3) Å is shorter than the corresponding value of 1.283 (3) Å observed in a similar Schiff base compound (Li *et al.*, 2006). The C7—N1—C8—C9 and N1—C8—C9—C10 torsion angles are −124.1 (2) and 98.2 (3)°, respectively. The dihedral angle between the two benzene rings is 71.6 (2)°. An intramolecular O—H···N hydrogen bond is formed between atoms O1 and N1 (Fig. 1 and Table 1).

Experimental

4-Fluorobenzylamine (125 mg, 1 mmol) and 5-chlorosalicylaldehyde (160 mg, 2 mmol) were dissolved in methanol (10 ml) at 323 K. The mixture was stirred for 10 min to give a clear yellow solution. After keeping the solution in air for 8 d, yellow block crystals were formed at the bottom of the vessel, in about 59% yield, on slow evaporation of the solvent. Elemental analysis found: C 63.76, H 4.23, N 5.45%; calculated: C 63.77, H 4.20, N 5.31%.

Crystal data

$C_{14}H_{11}ClFNO$
M_r = 263.69
Monoclinic, $P2_1/c$
a = 15.0408 (17) Å
b = 6.0375 (7) Å
c = 14.3943 (17) Å
β = 105.068 (2)°
V = 1262.2 (3) Å^3
Z = 4
D_x = 1.388 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 292 (2) K
Block, yellow
0.36 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.930, T_{max} = 0.942
10448 measured reflections
2875 independent reflections
1922 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.171
S = 1.06
2875 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0827P)^2 + 0.0486P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.88	2.601 (2)	147

All H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.93 and 0.97 Å for sp^2 and sp^3 C atoms, respectively, O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). Atom H1 of the hydroxy group was placed so as to form the best hydrogen bond to N1.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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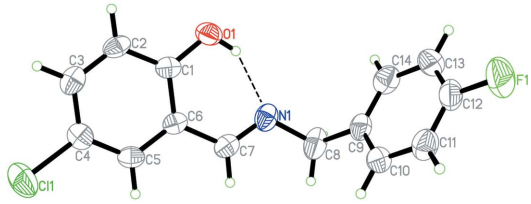

Figure 1
Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are shown at the 30% probability level. H atoms are shown as spheres of arbitrary radii. The dashed line denotes the intramolecular O—H···N hydrogen bond.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2003). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Erxleben, A. & Schumacher, D. (2001). *Eur. J. Inorg. Chem.* pp. 3039–3046.
Li, Y.-G., Zhu, H.-L., Chen, X.-Z. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m2385–m2387.
Li, Y.-G., Zhu, H.-L., Huang, W.-Q. & Ai, L. (2006). *Acta Cryst.* E**62**, o689–o690.
Mukhopadhyay, S., Mandal, D., Ghosh, D., Goldberg, I. & Chaudhury, M. (2003). *Inorg. Chem.* **42**, 8439–8445.
Ranford, J. D., Vittal, J. J., Wu, D.-Q. & Yang, X.-D. (1999). *Angew. Chem. Int. Ed.* **38**, 3498–3501.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Sreenivasulu, B., Vetrichelvan, M., Zhao, F., Gao, S. & Vittal, J. J. (2005). *Eur. J. Inorg. Chem.* pp. 4635–4645.