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2-(Cyclopropyliminomethyl)-4-nitrophenol

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.136
Data-to-parameter ratio = 14.5

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

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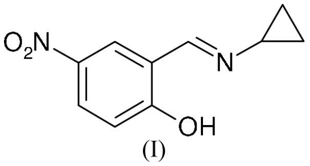
The title compound, $C_{10}H_{10}N_2O_3$, is a Schiff base compound derived from the condensation of equimolar 5-nitrosalicylaldeheyde and cyclopropylamine in MeOH. The molecule adopts a *trans* configuration about the C=N bond and there is an intramolecular O—H···N hydrogen bond.

Comment

Schiff base compounds derived from salicylaldehyde have been of great interest in coordination chemistry for many years (Nishijima *et al.*, 1995; Archer & Wang, 1990). They can easily coordinate to transition metal ions through the deprotonated phenolate O atoms and the imine N atoms. As part of an investigation of the crystal structures of such ligands, the structure of (I) is reported here.



(I)

Compound (I) is a Schiff base compound (Fig. 1), which is derived from the condensation of equimolar salicylaldehyde and cyclopropylamine in MeOH. All the bond lengths in the compound are within normal ranges (Allen *et al.*, 1987). As expected, the molecule adopts a *trans* configuration about the C7=N2 bond. The dihedral angle between the cyclopropane and benzene rings is 89.5 (2)°. The dihedral angle between the benzene ring and the O1/N1/O2 nitryl plane is 6.0 (2)°, probably due to the presence of an intramolecular O—H···N hydrogen bond (Table 1). In the crystal structure, there are no obviously short contacts (Fig. 2).

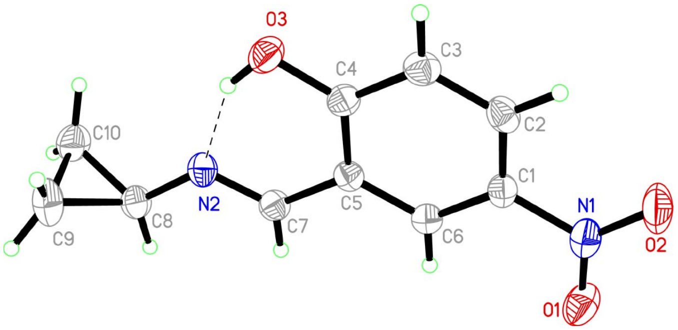


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

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Experimental

Salicylaldehyde (0.1 mmol, 12.1 mg) and cyclopropylamine (0.1 mmol, 5.7 mg) were dissolved in MeOH (10 ml). The mixture was stirred for 30 min to give a yellow solution. The solution was kept in air for 7 d and yellow block-shaped crystals were obtained.

Crystal data

$C_{10}H_{10}N_2O_3$
$M_r = 206.20$
Monoclinic, $P2_1/c$
$a = 7.800$ (2) Å
$b = 5.845$ (2) Å
$c = 21.610$ (3) Å
$\beta = 97.599$ (2)°
$V = 976.6$ (2) Å^3
$Z = 4$
$D_x = 1.402$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2043 reflections
$\theta = 2.6$–26.5°
$\mu = 0.11$ mm^{-1}
$T = 298$ (2) K
Block, yellow
0.25 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.974$, $T_{\max} = 0.985$
7544 measured reflections
2022 independent reflections
1694 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\max} = 26.5°$
$h = -9 \rightarrow 9$
$k = -7 \rightarrow 7$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.136$
$S = 1.13$
2022 reflections
139 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.2047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.32$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···N2	0.90 (1)	1.739 (15)	2.576 (2)	153 (2)

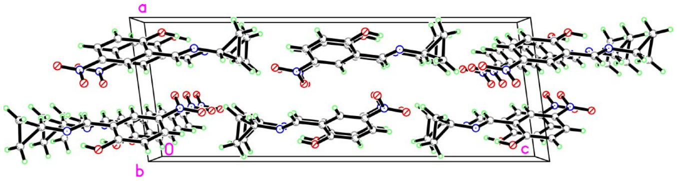

Figure 2
The crystal packing of (I), viewed along the *b* axis.

The hydroxyl atom H3 was located in a difference Fourier map and refined isotropically, with the O—H distance restrained to 0.90 (1) Å. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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