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# 2-Ethoxy-6-[(3-methylpyridin-2-yl)iminomethyl]phenol

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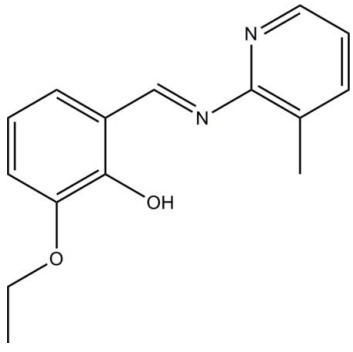
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.074; $wR$ factor = 0.200; data-to-parameter ratio = 16.3.

The title Schiff base compound, $C_{15}H_{16}N_2O_2$, was prepared by the condensation reaction of equimolar quantities of 3-ethoxysalicylaldehyde with 2-amino-3-methylpyridine in methanol. The dihedral angle between the benzene ring and the pyridine ring is 2.6 (2)° and an intramolecular O—H···N hydrogen bond generates an $S$(6) ring.

## Related literature

For background to Schiff bases, see: Sinha *et al.* (2008); Sonmez *et al.* (2010); Mohamed *et al.* (2010). For related structures, see: Wang & Shi (2008); Zhao *et al.* (2010); Karadağ *et al.* (2011); Bingöl Alpaslan *et al.* (2010).




## Experimental

### Crystal data

$C_{15}H_{16}N_2O_2$
$M_r$ = 256.30
Monoclinic, $P2_1/n$
$a$ = 4.820 (1) Å
$b$ = 38.385 (3) Å
$c$ = 7.207 (2) Å
$\beta$ = 96.381 (2)°
$V$ = 1325.1 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 K
0.17 × 0.15 × 0.15 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.985, $T_{max}$ = 0.987
7773 measured reflections
2849 independent reflections
1265 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.200
$S$ = 1.03
2849 reflections
175 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 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 | 1.87 | 2.590 (3) | 146 |

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5833).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o1064 [ **doi:10.1107/S1600536811012116** ]

# 2-Ethoxy-6-[(3-methylpyridin-2-yl)iminomethyl]phenol

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## Comment

Much effort has been paid on the preparation, structures, and applications of Schiff bases (Sinha *et al.*, 2008; Sonmez *et al.*, 2010; Mohamed *et al.*, 2010). As a continuation of the work on the crystal structures of Schiff bases, the title new Schiff base compound, Fig. 1, is reported.

The whole molecule of the compound is approximately planar, with a mean deviation from the least squares plane through all 19 non-hydrogen atoms of 0.036 (2) Å; the dihedral angle between the C1–C6 benzene ring and the C8–C12/N2 pyridine ring is 2.6 (2)°. There is an intramolecular O1—H1···N1 hydrogen bond (Table 1), which helps the formation of the planarity of the molecule. The bond lengths and angles are comparable to those found in the similar Schiff base compounds (Wang & Shi, 2008; Zhao *et al.*, 2010; Karadağ *et al.*, 2011; Bingöl Alpaslan *et al.*, 2010).

## Experimental

Reagents and solvents used were of commercially available quality. A methanol solution (10 ml) of 2-amino-3-methylpyridine (0.1 mmol, 10.8 mg) was added to a stirred methanol solution (10 ml) of 3-ethoxysalicylaldehyde (0.1 mmol, 16.6 mg). After stirring for about 30 min at room temperature, the clear yellow solution was left to stand still in air. Yellow block-shaped crystals of the title compound were formed after slow evaporation of the solvent for a few days.

## Refinement

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, O—H distance of 0.82 Å, and with $U_{iso}$(H) set to 1.2$U_{eq}$(C) and 1.5$U_{eq}$(O1, C13 and C15).

## Figures

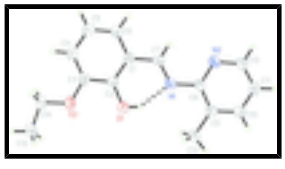

Fig. 1. Molecular structure of the title compound with 30% probability ellipsoids.

## 2-Ethoxy-6-[(3-methylpyridin-2-yl)iminomethyl]phenol

*Crystal data*

| | |
|---|---|
| $C_{15}H_{16}N_2O_2$ | $F(000) = 544$ |
| $M_r = 256.30$ | $D_x = 1.285$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |

| | |
|---|---|
| Hall symbol: -P 2yn | Cell parameters from 776 reflections |
| $a$ = 4.820 (1) Å | θ = 2.5–24.5° |
| $b$ = 38.385 (3) Å | μ = 0.09 $mm^{-1}$ |
| $c$ = 7.207 (2) Å | $T$ = 298 K |
| β = 96.381 (2)° | Block, yellow |
| $V$ = 1325.1 (5) $Å^3$ | 0.17 × 0.15 × 0.15 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2849 independent reflections |
| Radiation source: fine-focus sealed tube | 1265 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int}$ = 0.061 |
| ω scan | $\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.9° |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -6 \rightarrow 6$ |
| $T_{min}$ = 0.985, $T_{max}$ = 0.987 | $k = -49 \rightarrow 49$ |
| 7773 measured reflections | $l = -9 \rightarrow 9$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.074 | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2)$ = 0.200 | H-atom parameters constrained |
| $S$ = 1.03 | $w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 0.153P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2849 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 175 parameters | $\Delta\rho_{max}$ = 0.23 e $Å^{-3}$ |
| 0 restraints | $\Delta\rho_{min}$ = −0.18 e $Å^{-3}$ |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.6449 (5) | 0.84753 (6) | 0.0653 (4) | 0.0495 (7) |
| N2 | 0.9399 (6) | 0.80518 (7) | 0.2233 (4) | 0.0604 (8) |
| O1 | 0.3096 (5) | 0.89291 (6) | −0.1048 (3) | 0.0609 (7) |
| H1 | 0.4207 | 0.8767 | −0.0957 | 0.091* |
| O2 | −0.0665 (5) | 0.94125 (6) | −0.0911 (3) | 0.0691 (7) |
| C1 | 0.3479 (6) | 0.88351 (8) | 0.2257 (5) | 0.0508 (8) |
| C2 | 0.2310 (6) | 0.90021 (8) | 0.0638 (4) | 0.0458 (8) |
| C3 | 0.0320 (7) | 0.92615 (8) | 0.0768 (5) | 0.0550 (9) |
| C4 | −0.0520 (7) | 0.93435 (9) | 0.2466 (5) | 0.0656 (10) |
| H4 | −0.1876 | 0.9514 | 0.2543 | 0.079* |
| C5 | 0.0632 (8) | 0.91749 (10) | 0.4080 (5) | 0.0728 (11) |
| H5 | 0.0057 | 0.9234 | 0.5229 | 0.087* |
| C6 | 0.2592 (7) | 0.89243 (9) | 0.3978 (5) | 0.0625 (10) |
| H6 | 0.3351 | 0.8811 | 0.5058 | 0.075* |
| C7 | 0.5550 (7) | 0.85676 (8) | 0.2183 (5) | 0.0530 (9) |
| H7 | 0.6260 | 0.8458 | 0.3286 | 0.064* |
| C8 | 0.8476 (6) | 0.82108 (8) | 0.0640 (5) | 0.0482 (8) |
| C9 | 0.9424 (7) | 0.81326 (8) | −0.1071 (5) | 0.0504 (8) |
| C10 | 1.1400 (7) | 0.78743 (9) | −0.1066 (5) | 0.0603 (10) |
| H10 | 1.2096 | 0.7813 | −0.2174 | 0.072* |
| C11 | 1.2348 (7) | 0.77076 (9) | 0.0558 (6) | 0.0666 (10) |
| H11 | 1.3680 | 0.7532 | 0.0568 | 0.080* |
| C12 | 1.1299 (7) | 0.78039 (9) | 0.2162 (5) | 0.0653 (10) |
| H12 | 1.1950 | 0.7690 | 0.3263 | 0.078* |
| C13 | 0.8314 (7) | 0.83182 (9) | −0.2831 (4) | 0.0679 (10) |
| H13A | 0.9225 | 0.8231 | −0.3855 | 0.102* |
| H13B | 0.8669 | 0.8563 | −0.2689 | 0.102* |
| H13C | 0.6340 | 0.8279 | −0.3074 | 0.102* |
| C14 | −0.2849 (7) | 0.96607 (9) | −0.0914 (5) | 0.0684 (11) |
| H14A | −0.2220 | 0.9861 | −0.0165 | 0.082* |
| H14B | −0.4439 | 0.9559 | −0.0399 | 0.082* |
| C15 | −0.3642 (9) | 0.97670 (11) | −0.2899 (6) | 0.0961 (14) |
| H15A | −0.2014 | 0.9847 | −0.3428 | 0.144* |
| H15B | −0.4995 | 0.9951 | −0.2943 | 0.144* |
| H15C | −0.4427 | 0.9571 | −0.3600 | 0.144* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0489 (16) | 0.0531 (16) | 0.0459 (17) | 0.0050 (13) | 0.0022 (13) | 0.0040 (13) |
| N2 | 0.0553 (18) | 0.0665 (19) | 0.0593 (19) | 0.0105 (15) | 0.0065 (15) | 0.0123 (15) |
| O1 | 0.0654 (17) | 0.0663 (16) | 0.0507 (14) | 0.0180 (12) | 0.0054 (12) | 0.0023 (12) |
| O2 | 0.0625 (15) | 0.0719 (16) | 0.0740 (17) | 0.0234 (13) | 0.0129 (13) | 0.0121 (13) |
| C1 | 0.0462 (19) | 0.051 (2) | 0.054 (2) | 0.0012 (16) | 0.0037 (16) | −0.0032 (17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0430 (19) | 0.0484 (19) | 0.046 (2) | −0.0020 (15) | 0.0049 (16) | −0.0013 (15) |
| C3 | 0.047 (2) | 0.053 (2) | 0.065 (2) | 0.0026 (16) | 0.0078 (18) | 0.0068 (18) |
| C4 | 0.058 (2) | 0.064 (2) | 0.077 (3) | 0.0098 (18) | 0.018 (2) | −0.004 (2) |
| C5 | 0.074 (3) | 0.084 (3) | 0.064 (3) | 0.013 (2) | 0.022 (2) | −0.006 (2) |
| C6 | 0.065 (2) | 0.077 (2) | 0.045 (2) | 0.008 (2) | 0.0060 (18) | 0.0018 (19) |
| C7 | 0.056 (2) | 0.058 (2) | 0.0441 (19) | 0.0016 (17) | −0.0005 (17) | 0.0029 (16) |
| C8 | 0.0435 (19) | 0.0469 (19) | 0.053 (2) | 0.0002 (15) | 0.0015 (16) | 0.0034 (16) |
| C9 | 0.0461 (19) | 0.052 (2) | 0.052 (2) | −0.0050 (16) | 0.0003 (16) | 0.0011 (16) |
| C10 | 0.059 (2) | 0.061 (2) | 0.061 (2) | 0.0038 (18) | 0.0065 (19) | −0.0075 (18) |
| C11 | 0.059 (2) | 0.059 (2) | 0.082 (3) | 0.0140 (18) | 0.012 (2) | 0.004 (2) |
| C12 | 0.065 (2) | 0.069 (2) | 0.063 (2) | 0.016 (2) | 0.0108 (19) | 0.021 (2) |
| C13 | 0.073 (3) | 0.081 (3) | 0.049 (2) | 0.007 (2) | 0.0033 (19) | 0.0014 (19) |
| C14 | 0.051 (2) | 0.060 (2) | 0.094 (3) | 0.0129 (18) | 0.007 (2) | 0.006 (2) |
| C15 | 0.099 (3) | 0.091 (3) | 0.094 (3) | 0.045 (3) | −0.007 (3) | 0.008 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C7 | 1.279 (4) | C7—H7 | 0.9300 |
| N1—C8 | 1.410 (4) | C8—C9 | 1.394 (4) |
| N2—C12 | 1.326 (4) | C9—C10 | 1.375 (4) |
| N2—C8 | 1.332 (4) | C9—C13 | 1.500 (4) |
| O1—C2 | 1.342 (3) | C10—C11 | 1.367 (4) |
| O1—H1 | 0.8200 | C10—H10 | 0.9300 |
| O2—C3 | 1.378 (4) | C11—C12 | 1.363 (5) |
| O2—C14 | 1.420 (4) | C11—H11 | 0.9300 |
| C1—C2 | 1.394 (4) | C12—H12 | 0.9300 |
| C1—C6 | 1.399 (4) | C13—H13A | 0.9600 |
| C1—C7 | 1.437 (4) | C13—H13B | 0.9600 |
| C2—C3 | 1.393 (4) | C13—H13C | 0.9600 |
| C3—C4 | 1.368 (5) | C14—C15 | 1.496 (5) |
| C4—C5 | 1.392 (5) | C14—H14A | 0.9700 |
| C4—H4 | 0.9300 | C14—H14B | 0.9700 |
| C5—C6 | 1.356 (4) | C15—H15A | 0.9600 |
| C5—H5 | 0.9300 | C15—H15B | 0.9600 |
| C6—H6 | 0.9300 | C15—H15C | 0.9600 |
| C7—N1—C8 | 120.5 (3) | C10—C9—C13 | 121.7 (3) |
| C12—N2—C8 | 117.5 (3) | C8—C9—C13 | 121.6 (3) |
| C2—O1—H1 | 109.5 | C11—C10—C9 | 120.3 (3) |
| C3—O2—C14 | 117.8 (3) | C11—C10—H10 | 119.8 |
| C2—C1—C6 | 119.6 (3) | C9—C10—H10 | 119.8 |
| C2—C1—C7 | 121.0 (3) | C12—C11—C10 | 118.6 (3) |
| C6—C1—C7 | 119.3 (3) | C12—C11—H11 | 120.7 |
| O1—C2—C3 | 118.4 (3) | C10—C11—H11 | 120.7 |
| O1—C2—C1 | 122.2 (3) | N2—C12—C11 | 123.4 (3) |
| C3—C2—C1 | 119.3 (3) | N2—C12—H12 | 118.3 |
| C4—C3—O2 | 125.6 (3) | C11—C12—H12 | 118.3 |
| C4—C3—C2 | 120.0 (3) | C9—C13—H13A | 109.5 |
| O2—C3—C2 | 114.5 (3) | C9—C13—H13B | 109.5 |
| C3—C4—C5 | 120.7 (3) | H13A—C13—H13B | 109.5 |

| | | | |
|---|---|---|---|
| C3—C4—H4 | 119.7 | C9—C13—H13C | 109.5 |
| C5—C4—H4 | 119.7 | H13A—C13—H13C | 109.5 |
| C6—C5—C4 | 120.0 (3) | H13B—C13—H13C | 109.5 |
| C6—C5—H5 | 120.0 | O2—C14—C15 | 107.2 (3) |
| C4—C5—H5 | 120.0 | O2—C14—H14A | 110.3 |
| C5—C6—C1 | 120.4 (3) | C15—C14—H14A | 110.3 |
| C5—C6—H6 | 119.8 | O2—C14—H14B | 110.3 |
| C1—C6—H6 | 119.8 | C15—C14—H14B | 110.3 |
| N1—C7—C1 | 122.2 (3) | H14A—C14—H14B | 108.5 |
| N1—C7—H7 | 118.9 | C14—C15—H15A | 109.5 |
| C1—C7—H7 | 118.9 | C14—C15—H15B | 109.5 |
| N2—C8—C9 | 123.5 (3) | H15A—C15—H15B | 109.5 |
| N2—C8—N1 | 119.3 (3) | C14—C15—H15C | 109.5 |
| C9—C8—N1 | 117.2 (3) | H15A—C15—H15C | 109.5 |
| C10—C9—C8 | 116.6 (3) | H15B—C15—H15C | 109.5 |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.87 | 2.590 (3) | 146 |

**Fig. 1**