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2-[(4-Ethylphenyl)iminomethyl]-3,5-dimethoxyphenol

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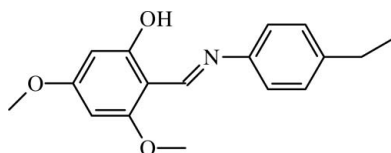
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.040; wR factor = 0.077; data-to-parameter ratio = 9.6.

The title compound, $\text{C}_{17}\text{H}_{19}\text{NO}_3$, adopts the phenol-imine tautomeric form, with a resonance-assisted $\text{O}-\text{H}\cdots\text{N}$ intramolecular hydrogen bond [$\text{O}\cdots\text{N} = 2.551$ (3) Å]. The dihedral angle between the two benzene rings is 45.42 (7)°. The two methoxy groups are coplanar with the attached benzene ring [$\text{C}-\text{O}-\text{C}-\text{C}$ torsion angles = -1.1 (5) and 3.2 (4)°].

Related literature

For the photochromic and thermochromic characteristics of Schiff base compounds, see: Hadjoudis *et al.* (1987); Lozier *et al.* (1975). For the notation of hydrogen-bonding motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_{17}\text{H}_{19}\text{NO}_3$
 $M_r = 285.33$

 Orthorhombic, $P2_12_12_1$
 $a = 7.5026$ (5) Å
 $b = 9.4540$ (8) Å
 $c = 21.4408$ (13) Å
 $V = 1520.79$ (19) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 296$ K
 $0.46 \times 0.35 \times 0.11$ mm

Data collection

 Stoe IPDS II diffractometer
 Absorption correction: integration
 ($X\text{-RED32}$; Stoe & Cie, 2002)
 $T_{\min} = 0.991$, $T_{\max} = 0.998$

 10094 measured reflections
 1831 independent reflections
 1036 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.077$
 $S = 0.92$
 1831 reflections

 191 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.09$ e Å⁻³
 $\Delta\rho_{\min} = -0.11$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------------|-------|-------------|-------------|---------------|
| $\text{O3}-\text{H3}\cdots\text{N1}$ | 0.82 | 1.82 | 2.551 (3) | 149 |

Data collection: $X\text{-AREA}$ (Stoe & Cie, 2002); cell refinement: $X\text{-AREA}$; data reduction: $X\text{-RED32}$ (Stoe & Cie, 2002); program(s) used to solve structure: $SHELXS97$ (Sheldrick, 2008); program(s) used to refine structure: $SHELXL97$ (Sheldrick, 2008); molecular graphics: $ORTEP-3$ for Windows (Farrugia, 1997); software used to prepare material for publication: $WinGX$ (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2762).

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supplementary materials

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2-[(4-Ethylphenyl)iminomethyl]-3,5-dimethoxyphenol

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Comment

Most Schiff base compounds have antibacterial, anticancer, anti-inflammatory and antioxic properties. In addition Schiff bases are important in diverse fields of chemistry and biochemistry owing to their biological activities (Lozier *et al.*, 1975). There are two types of intramolecular hydrogen bonds in Schiff bases which may stabilize them in keto–amine (N—H···O hydrogen bond) or phenol–imine (N···H—O hydrogen bond) tautomeric forms (Hadjoudis *et al.*, 1987). Our investigations show that the title compound adopts the phenol–imine tautomeric form (Fig. 1).

The N1—C7 bond length of 1.281 (3) Å is typical of a double bond. The dihedral angle between the C1—C6 and C8—C13 benzene rings is 45.4 (2)°. The C4—C7—N1—C8 torsion angle is -179.5 (3)°. The strong intramolecular O3—H3···N1 hydrogen bond forms an *S*(6) motif (Bernstein *et al.*, 1995).

Experimental

2-Hydroxy-4,6-dimethoxybenzaldehyde (0.0327 g, 0.18 mmol) in ethanol (20 ml) was added to a solution of 4-ethylaniline (0.0219 g, 0.18 mmol) in ethanol (20 ml) and the reaction mixture was stirred for 1 h under reflux, to obtain the title compound. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (yield 61%; m.p.351–353 K).

Refinement

All H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å, O—H = 0.82 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{C}_{\text{methyl}}, \text{O})$. In the absence of significant anomalous dispersion effects, Friedel pairs were merged before the final refinement.

Figures

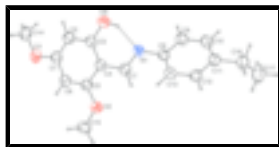


Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability.

2-[(4-Ethylphenyl)iminomethyl]-3,5-dimethoxyphenol

Crystal data

$\text{C}_{17}\text{H}_{19}\text{NO}_3$
 $M_r = 285.33$

$F_{000} = 608$
 $D_x = 1.246 \text{ Mg m}^{-3}$

supplementary materials

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 7.5026$ (5) Å

$b = 9.4540$ (8) Å

$c = 21.4408$ (13) Å

$V = 1520.79$ (19) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 10094 reflections

$\theta = 1.9$ – 27.7°

$\mu = 0.09$ mm⁻¹

$T = 296$ K

Prism, yellow

$0.46 \times 0.35 \times 0.11$ mm

Data collection

Stoe IPDS II

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 6.67 pixels mm⁻¹

$T = 296$ K

ω scans

Absorption correction: integration

(X-RED32; Stoe & Cie, 2002)

$T_{\min} = 0.991$, $T_{\max} = 0.998$

10094 measured reflections

1831 independent reflections

1036 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.049$

$\theta_{\text{max}} = 26.5^\circ$

$\theta_{\text{min}} = 1.9^\circ$

$h = -9 \rightarrow 8$

$k = -11 \rightarrow 10$

$l = -26 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.077$

$S = 0.92$

1831 reflections

191 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0332P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.09$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.11$ e Å⁻³

Extinction correction: none

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|------------|-------------|--------------|----------------------------------|
| C1 | 0.2906 (4) | 0.3417 (3) | 0.70797 (12) | 0.0630 (8) |
| C2 | 0.2290 (5) | 0.3445 (3) | 0.76807 (12) | 0.0692 (9) |
| H2 | 0.1988 | 0.4295 | 0.7871 | 0.083* |
| C3 | 0.2128 (4) | 0.2174 (3) | 0.79972 (12) | 0.0635 (8) |
| C4 | 0.2526 (4) | 0.0871 (3) | 0.77182 (11) | 0.0566 (7) |
| C5 | 0.3141 (4) | 0.0911 (3) | 0.70914 (12) | 0.0610 (8) |
| C6 | 0.3354 (4) | 0.2165 (3) | 0.67808 (12) | 0.0630 (8) |
| H6 | 0.3794 | 0.2178 | 0.6375 | 0.076* |
| C7 | 0.2409 (4) | -0.0436 (3) | 0.80628 (12) | 0.0601 (7) |
| H7 | 0.2663 | -0.1284 | 0.7862 | 0.072* |
| C8 | 0.1874 (4) | -0.1759 (3) | 0.89708 (11) | 0.0559 (7) |
| C9 | 0.2513 (4) | -0.1775 (3) | 0.95769 (12) | 0.0679 (8) |
| H9 | 0.2991 | -0.0956 | 0.9749 | 0.081* |
| C10 | 0.2447 (5) | -0.3000 (3) | 0.99269 (12) | 0.0699 (8) |
| H10 | 0.2930 | -0.3004 | 1.0326 | 0.084* |
| C11 | 0.1679 (4) | -0.4216 (3) | 0.96967 (12) | 0.0625 (8) |
| C12 | 0.1013 (4) | -0.4181 (3) | 0.90983 (12) | 0.0634 (8) |
| H12 | 0.0481 | -0.4988 | 0.8934 | 0.076* |
| C13 | 0.1118 (4) | -0.2971 (3) | 0.87352 (11) | 0.0604 (8) |
| H13 | 0.0675 | -0.2980 | 0.8330 | 0.072* |
| C14 | 0.2705 (5) | 0.5932 (3) | 0.69842 (14) | 0.0878 (10) |
| H14A | 0.2939 | 0.6663 | 0.6685 | 0.132* |
| H14B | 0.3412 | 0.6091 | 0.7350 | 0.132* |
| H14C | 0.1464 | 0.5944 | 0.7094 | 0.132* |
| C15 | 0.4190 (5) | -0.0439 (4) | 0.62229 (12) | 0.0884 (11) |
| H15A | 0.4361 | -0.1407 | 0.6102 | 0.133* |
| H15B | 0.5311 | 0.0049 | 0.6212 | 0.133* |
| H15C | 0.3372 | 0.0007 | 0.5940 | 0.133* |
| C16 | 0.1567 (5) | -0.5544 (3) | 1.00901 (14) | 0.0857 (10) |
| H16A | 0.1075 | -0.5299 | 1.0494 | 0.103* |
| H16B | 0.0747 | -0.6198 | 0.9892 | 0.103* |
| C17 | 0.3298 (6) | -0.6273 (4) | 1.01865 (17) | 0.1268 (16) |
| H17A | 0.3789 | -0.6538 | 0.9790 | 0.190* |
| H17B | 0.3116 | -0.7105 | 1.0435 | 0.190* |
| H17C | 0.4108 | -0.5648 | 1.0397 | 0.190* |
| N1 | 0.1964 (3) | -0.0451 (2) | 0.86397 (10) | 0.0629 (7) |
| O1 | 0.3148 (3) | 0.4591 (2) | 0.67216 (8) | 0.0834 (7) |
| O2 | 0.3479 (3) | -0.0388 (2) | 0.68417 (8) | 0.0781 (6) |
| O3 | 0.1587 (4) | 0.2229 (2) | 0.85970 (8) | 0.0879 (7) |
| H3 | 0.1526 | 0.1425 | 0.8738 | 0.132* |

Atomic displacement parameters (\AA^2)

U^{11} U^{22} U^{33} U^{12} U^{13} U^{23}

supplementary materials

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.063 (2) | 0.060 (2) | 0.0665 (18) | -0.0127 (18) | -0.0040 (17) | 0.0093 (15) |
| C2 | 0.082 (2) | 0.0589 (19) | 0.0672 (18) | -0.0111 (18) | 0.0035 (17) | -0.0034 (15) |
| C3 | 0.070 (2) | 0.0659 (18) | 0.0548 (15) | -0.0106 (19) | 0.0023 (15) | -0.0011 (15) |
| C4 | 0.0569 (19) | 0.0566 (18) | 0.0563 (15) | -0.0072 (17) | -0.0013 (14) | 0.0015 (14) |
| C5 | 0.059 (2) | 0.0607 (19) | 0.0630 (17) | 0.0015 (17) | -0.0005 (14) | -0.0030 (15) |
| C6 | 0.062 (2) | 0.0680 (19) | 0.0586 (15) | -0.0035 (19) | 0.0001 (14) | 0.0062 (16) |
| C7 | 0.0531 (18) | 0.0607 (18) | 0.0665 (17) | 0.0020 (17) | 0.0004 (15) | 0.0003 (14) |
| C8 | 0.0524 (19) | 0.062 (2) | 0.0534 (15) | 0.0002 (17) | 0.0044 (14) | 0.0009 (14) |
| C9 | 0.074 (2) | 0.067 (2) | 0.0621 (16) | -0.0129 (18) | -0.0080 (16) | -0.0051 (15) |
| C10 | 0.075 (2) | 0.078 (2) | 0.0569 (15) | -0.0050 (19) | -0.0071 (15) | 0.0078 (16) |
| C11 | 0.061 (2) | 0.062 (2) | 0.0642 (17) | 0.0031 (18) | 0.0066 (14) | 0.0035 (15) |
| C12 | 0.067 (2) | 0.0563 (19) | 0.0664 (18) | -0.0047 (17) | 0.0065 (16) | -0.0045 (15) |
| C13 | 0.059 (2) | 0.068 (2) | 0.0541 (15) | -0.0018 (17) | 0.0005 (14) | -0.0004 (16) |
| C14 | 0.104 (3) | 0.062 (2) | 0.097 (2) | -0.006 (2) | -0.009 (2) | 0.0148 (18) |
| C15 | 0.110 (3) | 0.092 (2) | 0.0636 (18) | 0.001 (2) | 0.0264 (18) | -0.0078 (17) |
| C16 | 0.100 (3) | 0.076 (2) | 0.081 (2) | 0.003 (2) | 0.0076 (19) | 0.0194 (18) |
| C17 | 0.125 (4) | 0.119 (3) | 0.137 (3) | 0.047 (3) | 0.038 (3) | 0.058 (3) |
| N1 | 0.0689 (18) | 0.0643 (15) | 0.0554 (14) | -0.0059 (15) | 0.0017 (12) | 0.0050 (11) |
| O1 | 0.1059 (19) | 0.0655 (13) | 0.0788 (14) | -0.0060 (14) | 0.0029 (12) | 0.0146 (12) |
| O2 | 0.0968 (17) | 0.0701 (14) | 0.0674 (12) | 0.0057 (13) | 0.0197 (12) | 0.0004 (11) |
| O3 | 0.136 (2) | 0.0651 (13) | 0.0621 (11) | -0.0094 (16) | 0.0212 (12) | -0.0037 (9) |

Geometric parameters (Å, °)

| | | | |
|----------|-----------|-------------|-----------|
| C1—O1 | 1.362 (3) | C11—C12 | 1.377 (3) |
| C1—C2 | 1.369 (3) | C11—C16 | 1.515 (4) |
| C1—C6 | 1.387 (4) | C12—C13 | 1.386 (4) |
| C2—C3 | 1.385 (4) | C12—H12 | 0.93 |
| C2—H2 | 0.93 | C13—H13 | 0.93 |
| C3—O3 | 1.350 (3) | C14—O1 | 1.426 (3) |
| C3—C4 | 1.401 (3) | C14—H14A | 0.96 |
| C4—C5 | 1.421 (3) | C14—H14B | 0.96 |
| C4—C7 | 1.442 (3) | C14—H14C | 0.96 |
| C5—O2 | 1.364 (3) | C15—O2 | 1.430 (3) |
| C5—C6 | 1.370 (4) | C15—H15A | 0.96 |
| C6—H6 | 0.93 | C15—H15B | 0.96 |
| C7—N1 | 1.281 (3) | C15—H15C | 0.96 |
| C7—H7 | 0.93 | C16—C17 | 1.485 (5) |
| C8—C13 | 1.375 (4) | C16—H16A | 0.97 |
| C8—C9 | 1.385 (3) | C16—H16B | 0.97 |
| C8—N1 | 1.428 (3) | C17—H17A | 0.96 |
| C9—C10 | 1.381 (4) | C17—H17B | 0.96 |
| C9—H9 | 0.93 | C17—H17C | 0.96 |
| C10—C11 | 1.377 (4) | O3—H3 | 0.82 |
| C10—H10 | 0.93 | | |
| O1—C1—C2 | 124.0 (3) | C11—C12—H12 | 119.2 |
| O1—C1—C6 | 113.7 (2) | C13—C12—H12 | 119.2 |
| C2—C1—C6 | 122.2 (3) | C8—C13—C12 | 120.3 (2) |
| C1—C2—C3 | 118.3 (3) | C8—C13—H13 | 119.8 |

| | | | |
|---------------|------------|-----------------|------------|
| C1—C2—H2 | 120.9 | C12—C13—H13 | 119.8 |
| C3—C2—H2 | 120.9 | O1—C14—H14A | 109.5 |
| O3—C3—C2 | 117.4 (3) | O1—C14—H14B | 109.5 |
| O3—C3—C4 | 120.3 (3) | H14A—C14—H14B | 109.5 |
| C2—C3—C4 | 122.3 (2) | O1—C14—H14C | 109.5 |
| C3—C4—C5 | 116.7 (3) | H14A—C14—H14C | 109.5 |
| C3—C4—C7 | 121.4 (2) | H14B—C14—H14C | 109.5 |
| C5—C4—C7 | 121.8 (3) | O2—C15—H15A | 109.5 |
| O2—C5—C6 | 124.5 (2) | O2—C15—H15B | 109.5 |
| O2—C5—C4 | 114.1 (2) | H15A—C15—H15B | 109.5 |
| C6—C5—C4 | 121.4 (3) | O2—C15—H15C | 109.5 |
| C5—C6—C1 | 119.0 (3) | H15A—C15—H15C | 109.5 |
| C5—C6—H6 | 120.5 | H15B—C15—H15C | 109.5 |
| C1—C6—H6 | 120.5 | C17—C16—C11 | 114.4 (3) |
| N1—C7—C4 | 121.3 (3) | C17—C16—H16A | 108.7 |
| N1—C7—H7 | 119.3 | C11—C16—H16A | 108.7 |
| C4—C7—H7 | 119.3 | C17—C16—H16B | 108.7 |
| C13—C8—C9 | 118.6 (3) | C11—C16—H16B | 108.7 |
| C13—C8—N1 | 124.0 (2) | H16A—C16—H16B | 107.6 |
| C9—C8—N1 | 117.3 (3) | C16—C17—H17A | 109.5 |
| C10—C9—C8 | 120.4 (3) | C16—C17—H17B | 109.5 |
| C10—C9—H9 | 119.8 | H17A—C17—H17B | 109.5 |
| C8—C9—H9 | 119.8 | C16—C17—H17C | 109.5 |
| C11—C10—C9 | 121.4 (3) | H17A—C17—H17C | 109.5 |
| C11—C10—H10 | 119.3 | H17B—C17—H17C | 109.5 |
| C9—C10—H10 | 119.3 | C7—N1—C8 | 120.1 (2) |
| C10—C11—C12 | 117.8 (3) | C1—O1—C14 | 118.1 (2) |
| C10—C11—C16 | 121.0 (3) | C5—O2—C15 | 117.6 (2) |
| C12—C11—C16 | 121.2 (3) | C3—O3—H3 | 109.5 |
| C11—C12—C13 | 121.5 (3) | | |
| O1—C1—C2—C3 | -179.1 (3) | N1—C8—C9—C10 | 179.2 (3) |
| C6—C1—C2—C3 | 0.5 (5) | C8—C9—C10—C11 | -2.9 (5) |
| C1—C2—C3—O3 | 177.4 (3) | C9—C10—C11—C12 | 1.5 (5) |
| C1—C2—C3—C4 | -1.8 (5) | C9—C10—C11—C16 | -178.3 (3) |
| O3—C3—C4—C5 | -178.1 (3) | C10—C11—C12—C13 | 0.4 (4) |
| C2—C3—C4—C5 | 1.1 (4) | C16—C11—C12—C13 | -179.7 (3) |
| O3—C3—C4—C7 | -1.4 (4) | C9—C8—C13—C12 | -0.4 (4) |
| C2—C3—C4—C7 | 177.8 (3) | N1—C8—C13—C12 | -177.1 (3) |
| C3—C4—C5—O2 | -179.0 (3) | C11—C12—C13—C8 | -1.0 (4) |
| C7—C4—C5—O2 | 4.3 (4) | C10—C11—C16—C17 | -71.9 (4) |
| C3—C4—C5—C6 | 0.8 (4) | C12—C11—C16—C17 | 108.2 (4) |
| C7—C4—C5—C6 | -175.8 (3) | C4—C7—N1—C8 | -179.5 (3) |
| O2—C5—C6—C1 | 177.8 (3) | C13—C8—N1—C7 | -43.7 (4) |
| C4—C5—C6—C1 | -2.1 (4) | C9—C8—N1—C7 | 139.6 (3) |
| O1—C1—C6—C5 | -179.0 (3) | C2—C1—O1—C14 | -1.1 (5) |
| C2—C1—C6—C5 | 1.4 (5) | C6—C1—O1—C14 | 179.3 (3) |
| C3—C4—C7—N1 | -1.1 (4) | C6—C5—O2—C15 | 3.2 (4) |
| C5—C4—C7—N1 | 175.4 (3) | C4—C5—O2—C15 | -176.9 (3) |
| C13—C8—C9—C10 | 2.3 (5) | | |

supplementary materials

Hydrogen-bond geometry (Å, °)

| | | | | |
|-------------------------|-------------|---------------|-----------------------|-------------------------|
| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
| O3—H3···N1 | 0.82 | 1.82 | 2.551 (3) | 149 |

Fig. 1

