Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(*E*)-2-{1-[(4-Ethoxyphenyl)imino]ethyl}phenol

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Received 13 December 2006
Accepted 16 January 2007

The crystal structure of the title compound, $C_{16}H_{17}NO_2$, contains two independent molecules in the asymmetric unit. Both molecules adopt the phenol–imine tautomeric form, with strong intramolecular O—H···N hydrogen bonds. The crystal packing is stabilized by van der Waals interactions.

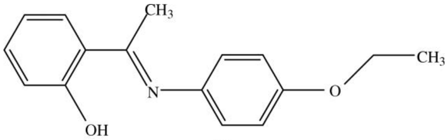
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.116
Data-to-parameter ratio = 13.6

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

Comment

Schiff bases and their complexes are of great interest in many fields of chemistry and biochemistry with respect to their significant antitumour activities (Zhou *et al.*, 2000). Schiff bases can be classified by their photochromic and thermochromic properties (Cohen *et al.*, 1964). Photochromism and thermochromism are produced by the reversible intramolecular proton transfer associated with a change in π-electron configuration (Hadjoudis *et al.*, 1987). In general, there are two tautomeric forms of Schiff bases; phenol–imine (OH form) and keto–amine (NH form), in which the proton is located at the O and N atom, respectively. Another tautomeric form of Schiff base compounds is the zwitterionic form with an ionic intramolecular hydrogen bond N^+—H···O^- (Ogawa & Harada, 2003; Petek *et al.*, 2006).



(I)

The two molecules of the asymmetric unit, *a* and *b* (Fig. 1), have very similar geometrical parameters, and the structure is pseudo-*C* centred. The r.m.s deviations associated with the bond distances and angles are 0.0033 Å and 0.233°, respectively. The C7*a*—N1*a* [1.2889 (15) Å] and C7*b*—N1*b* [1.2891 (14) Å] bond distances are of double-bond character, whereas the C1*a*—O1*a* [1.3486 (16) Å] and C1*b*—O1*b* [1.3443 (15) Å] distances are of single-bond character. When comparing these bonds with their corresponding values previously reported in the literature, it can be stated that both molecules in the asymmetric unit adopt the phenol–imine tautomeric form [C═N = 1.280 (3) and C—O = 1.347 (3) Å; Ünver *et al.*, 2002]. Molecules *a* and *b* are not planar: the dihedral angle between the C1*a*–C6*a* and C9*a*–C14*a* rings and the analogue in *b* are 64.63 (4) and 66.31 (4)°, respectively. The crystal packing is stabilized by van der Waals interactions.

Experimental

(*E*)-2-[1-(4-Ethoxyphenylimino)ethyl]phenol was prepared by reflux of a solution mixture containing 2-hydroxyacetophenone (1 g, 7.3 mmol) in methanol (20 ml) and a solution containing 4-ethoxyaniline (1 g, 7.3 mmol) in methanol (20 ml). The reaction mixture was stirred for 24 h under reflux. The resulting yellow precipitate was filtered off and crystals of (*E*)-2-[1-(4-ethoxyphenylimino)ethyl]phenol suitable for X-ray analysis were obtained from ethanol by slow evaporation (yield 23%; m.p. 251–253 K).

Crystal data

$C_{16}H_{17}NO_2$
$M_r = 255.31$
Triclinic, $P\overline{1}$
$a = 9.0671\ (7)$ Å
$b = 11.1923\ (8)$ Å
$c = 14.8312\ (12)$ Å
$\alpha = 86.037\ (6)^\circ$
$\beta = 75.742\ (6)^\circ$
$\gamma = 71.119\ (6)^\circ$
$V = 1380.15\ (18)$ Å^3
$Z = 4$
$D_x = 1.229$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Prism, yellow
0.75 × 0.60 × 0.36 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: none
22614 measured reflections
6540 independent reflections
3807 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.042$
$\theta_{\rm max} = 27.9^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.116$
$S = 0.99$
6540 reflections
480 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.12$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.11$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0189 (17)

Table 1
Selected geometric parameters (Å, °).

C6*b*—C7*b*	1.4689 (16)	C6*a*—C7*a*	1.4681 (17)
C9*b*—N1*b*	1.4200 (15)	C9*a*—N1*a*	1.4157 (16)
C12*b*—O2*b*	1.3706 (14)	C12*a*—O2*a*	1.3665 (15)
C15*b*—O2*b*	1.4228 (15)	C15*a*—O2*a*	1.4240 (16)
C15*b*—C16*b*	1.489 (2)	C15*a*—C16*a*	1.491 (2)
O2*b*—C15*b*—C16*b*	107.75 (12)	O2*a*—C15*a*—C16*a*	107.67 (13)
C12*b*—O2*b*—C15*b*	118.41 (9)	C12*a*—O2*a*—C15*a*	118.71 (9)
C6*b*—C7*b*—N1*b*—C9*b*	177.59 (10)	C6*a*—C7*a*—N1*a*—C9*a*	178.67 (10)
C16*b*—C15*b*—O2*b*—C12*b*	−178.64 (11)	C16*a*—C15*a*—O2*a*—C12*a*	−174.56 (12)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*b*—H1*b*···N1*b*	0.957 (16)	1.681 (16)	2.5420 (14)	147.7 (13)
O1*a*—H1*a*···N1*a*	1.06 (2)	1.55 (2)	2.5415 (14)	152.3 (18)

All H atoms were located in a difference Fourier map and were refined independently with isotropic displacement parameters. C—H distances are in the range 0.924 (16)–1.04 (1) Å and $U_{\rm iso}$(H) values are in the range 0.062 (3)–0.143 (7) Å^2.

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

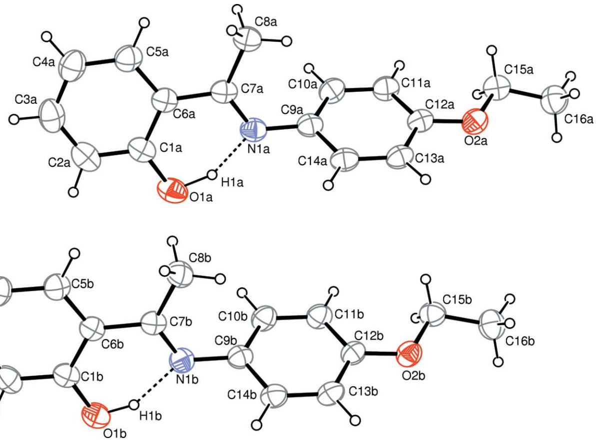


Figure 1
The asymmetric unit of (I), with the atom-numbering scheme and displacement ellipsoids at the 30% probability level. Dashed lines indicate hydrogen bonds.

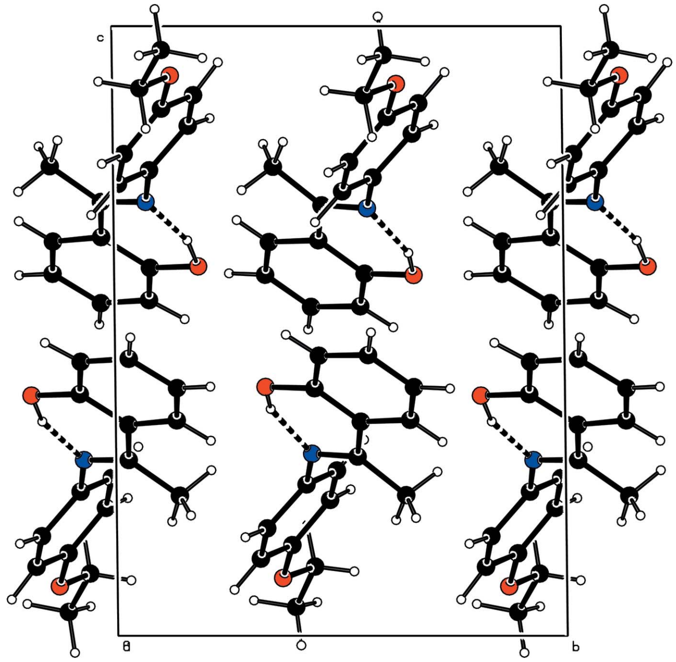


Figure 2
The crystal packing of (I), viewed down the *a* axis. Dashed lines indicate intramolecular hydrogen bonds.

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS II diffractometer (purchased under grants F.279 of the University Research Fund).

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