(E)-2-Hydroxy-3-methoxy-5-[(4-propylphenyl)diazenyl]benzaldehyde

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Key indicators

Single-crystal X-ray study
$T = 296$ K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.059
Data-to-parameter ratio = 14.1

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

In the title compound, $C_{18}H_{20}N_2O_3$, the azobenzene unit has a *trans* configuration, and the two benzene rings are inclined with respect to each other by 5.9 (2)°. Molecules are linked by O—H···O hydrogen bonds into a linear chain along [10$\bar{1}$].

Comment

Azo compounds have attracted great interest in organic synthesis. In the class of dye molecules, azo compounds are an important type of organic colorants and consist of at least a conjugated chromophore azo group and two or more aromatic rings. The colour of an azo dye is mainly due to the interaction of the azo group with incident light. Azo dyes are widely used in textiles, printing, cosmetics, drugs, food colouring and other consumer goods (Russ & Tappe, 1994; Tsuda *et al.*, 2000). We report here the structure of the title compound, (I).

(I)
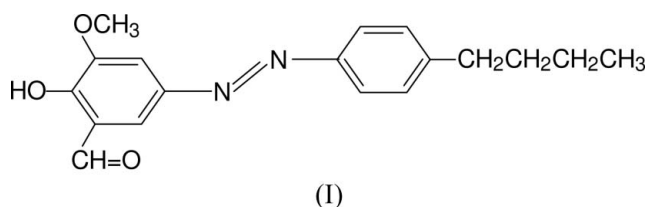
The molecular structure of (I) is shown in Fig. 1, with the atom-numbering scheme. The benzene rings adopt a *trans* configuration about the azo functional group. The A/B, A/C, C/B and B/D dihedral angles between the planes A (C7–C12), B (C1–C6), C (C1/N1/N2/C7) and D (C15–C18) are 5.9 (2), 11.0 (3), 5.3 (3) and 65.5 (2)°, respectively.

All the C—C bond lengths in the C1–C6 and C7–C12 benzene rings have typical Csp^2—Csp^2 values. The average C—C bond lengths within these two rings are 1.375 (3) and 1.385 (3) Å, respectively. The N1═N2 bond length of 1.250 (2) Å is almost equal to those found for similar compounds [1.256 (2) Å (Odabaşoğlu *et al.*, 2003), 1.252 (2) Å (Karadayı *et al.*, 2006*a*), and 1.255 (2) Å (Karadayı *et al.*, 2006*b*)]. The C9—C13, C10—O3 and C11—O4 bond lengths are 1.460 (3), 1.357 (3) and 1.357 (3) Å, respectively, and these values are comparable with those observed in our previous studies [1.445 (3), 1.350 (2) and 1.356 (2) Å (Karadayı *et al.*, 2006*a*), and 1.447 (3), 1.349 (2) and 1.355 (2) Å (Karadayı *et al.*, 2006*b*)]. An intramolecular O—H···O hydrogen bond is present in the molecule.

In the crystal structure of (I), intermolecular O—H···O hydrogen bonds (Table 1) generate a chain along [10$\bar{1}$].

Experimental

Compound (I) was prepared according to the literature method of Odabaşoğlu *et al.* (2003), using 4-*n*-butylaniline and *o*-vanillin as starting materials. Suitable single crystals of (I) were obtained by slow evaporation of an acetic acid solution (yield 87%; m.p. 367–369 K).

Crystal data

$C_{18}H_{20}N_2O_3$
$M_r = 312.36$
Monoclinic, $P2_1/n$
$a = 4.6264\ (10)$ Å
$b = 35.911\ (7)$ Å
$c = 10.342\ (2)$ Å
$\beta = 101.974\ (16)°$
$V = 1680.9\ (6)$ Å^3

$Z = 4$
$D_x = 1.234$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 296\ (2)$ K
Plate, brown
$0.37 \times 0.29 \times 0.07$ mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration
(X-$RED32$; Stoe & Cie, 2002)
$T_{min} = 0.972$, $T_{max} = 0.989$

10696 measured reflections
2983 independent reflections
831 reflections with $I > 2\sigma(I)$
$R_{int} = 0.079$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.059$
$S = 0.80$
2983 reflections
211 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0064P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0047 (5)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3$\cdots$O4	0.82	2.19	2.646 (2)	115
O3—H3$\cdots$O2^i	0.82	1.95	2.685 (2)	148

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$.

H atoms were positioned geometrically and refined using a riding model, with O—H = 0.82 Å, C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.5U_{eq}(C,O)$ for methyl and hydroxyl H atoms and $1.2U_{eq}(C)$ for
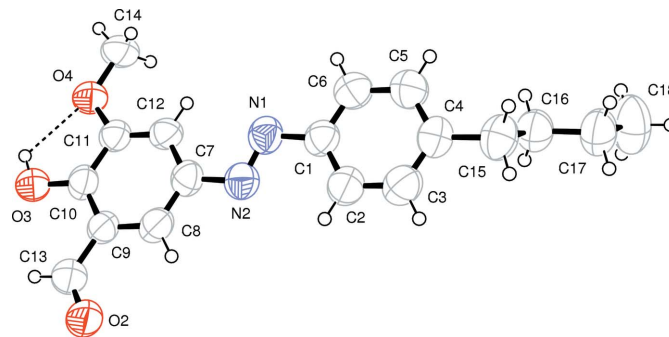

Figure 1
A view of (I), showing the atomic numbering scheme and 50% probability displacement ellipsoids. The intramolecular hydrogen bond is shown as a dashed line.

others. A rotating-group model was used for the hydroxyl and methyl groups.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (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) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Karadayı, N., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2006a). *Acta Cryst.* E**62**, o1699–o1701.
Karadayı, N., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2006b). *Acta Cryst.* E**62**, o1727–o1729.
Odabaşoğlu, M., Albayrak, Ç., Büyükgüngör, O. & Goesmann, H. (2003). *Acta Cryst.* C**59**, o234–o236.
Russ, H. W. & Tappe, H. (1994). Eur. Pat. Appl. EP 629 627.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
Tsuda, S., Matsusaka, N., Madarame, H., Ueno, S., Susa, N., Ishida, K., Kawamura, N., Sekihashi, K. & Sasaki, Y. E. (2000). *Mutat. Res. Genet. Toxicol. Environ. Mutagenesis*, **465**, 11–26.