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(*E*)-1-[3-Ethoxy-4-(4-methylbenzenesulfonyloxy)-benzylidene]-2-(4-nitrophenyl)hydrazine acetonitrile solvate

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In the title compound, $C_{24}H_{24}N_4O_6S$, the ethylvanillin group makes dihedral angles of 59.15 (9) and 5.36 (8)° with the terminal 4-methylbenzene ring and the phenylhydrazine mean plane, respectively. The crystal structure is stabilized by intermolecular N—H···N hydrogen bonds and weak non-classical intermolecular C—H···O hydrogen-bonding interactions.

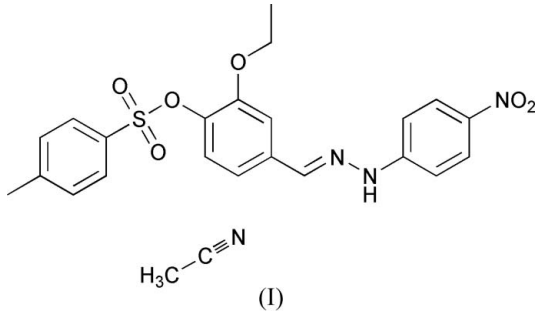
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.130
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

Metal complexes based on Schiff bases have attracted much attention because of their biological activity (Kahwa *et al.*, 1986). Consequently, a large number of Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics, such as models to mimic hydrolase in the hydrolysis of *p*-nitrophenyl picolinate (Li *et al.*, 2005). 1-(4-Nitrophenyl)hydrazine forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures of some of them, such as (*E*)-1-[4-(benzyloxy)benzylidene]-2-(4-nitrophenyl)hydrazine (Jun, 2005) and (*E*)-1-(4-methoxy-3-propoxybenzylidene)-2-(4-nitrophenyl)hydrazine (Shi, 2005), have been reported.



(I)

In the present study we report the synthesis and molecular structure of the nitrophenylhydrazine Schiff base derivative (I). In (I) (Fig. 1), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The phenylhydrazine residue (C17–C22/N1–N3) is planar, with an r.m.s. deviation for fitted atoms of 0.0168 Å. This plane makes dihedral angles of 45.93 (9) and 11.68 (8)° with the C1–C6 benzene ring and the ethylvanillin group (C8–C13/C16/O1/O4), respectively. The dihedral angle between the C1–C6 benzene ring and the vanillin group is 40.35 (7)°. The nitro group (O5/N3/O6) and its attached aromatic ring are not coplanar, with a dihedral angle of 9.70 (4)°.

An intermolecular N—H···N hydrogen bond helps to consolidate the crystal packing (Table 1 and Fig. 2). There is also a weak C—H···O intramolecular hydrogen-bonding

interaction, linking the main molecule and the solvent molecule.

Experimental

An anhydrous ethanol solution (50 ml) of 2-ethoxy-4-formylphenyl 4-methylbenzenesulfonate (3.20 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 1-(4-nitrophenyl)hydrazine (1.53 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen, giving a yellow precipitate. The product was isolated and recrystallized from acetonitrile. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{22}H_{21}N_3O_6S\cdot C_2H_3N$
$M_r = 496.54$
Triclinic, $P\overline{1}$
$a = 7.7257$ (17) Å
$b = 7.8019$ (18) Å
$c = 21.900$ (5) Å
$\alpha = 80.149$ (4)°
$\beta = 88.949$ (4)°
$\gamma = 72.208$ (3)°
$V = 1237.6$ (5) Å^3
$Z = 2$
$D_x = 1.332$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.18$ mm^{-1}
$T = 294$ (2) K
Block, yellow
0.28 × 0.26 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.937$, $T_{max} = 0.965$
6313 measured reflections
4332 independent reflections
3137 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.130$
$S = 1.06$
4332 reflections
319 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.202P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N4^{i}	0.86	2.25	3.094 (4)	167
C24—H24A···O2	0.96	2.54	3.229 (3)	129

Symmetry code: (i) $x-1, y, z$.

H atoms were included in calculated positions and refined using a riding-model approximation: C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2; C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene; C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl; N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) for amino H.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

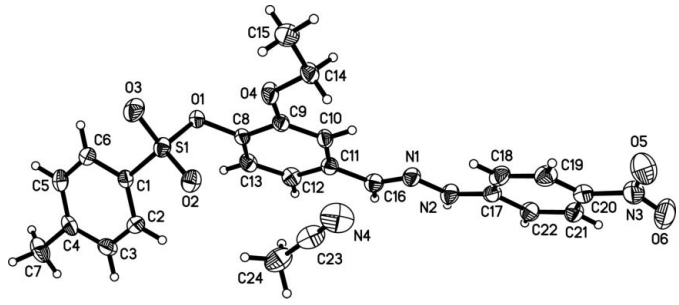


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

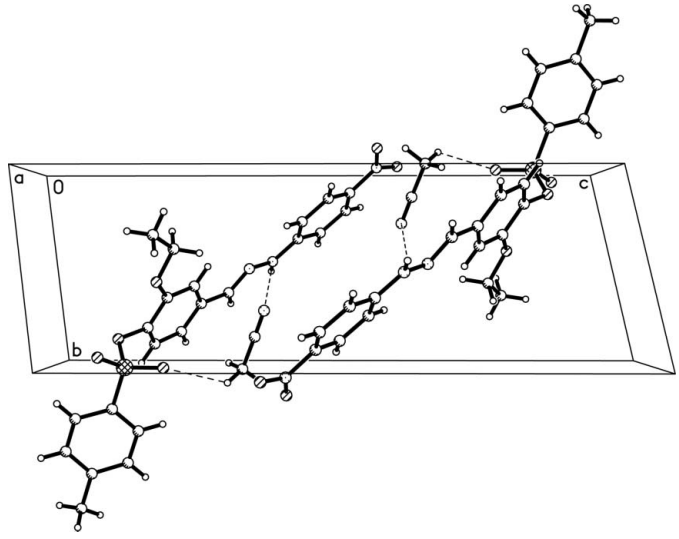


Figure 2
Packing diagram for (I), with hydrogen bonds drawn as dashed lines.

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