Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Ethoxy-4-formylphenyl benzenesulfonate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.118
Data-to-parameter ratio = 13.6

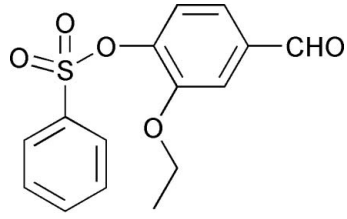
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 November 2006
Accepted 2 December 2006

In the title compound, $C_{15}H_{14}O_5S$, the ethylvanillin group makes a dihedral angle of 43.97 (8)° with the phenyl ring. The packing is stabilized by weak non-classical intermolecular C—H···O hydrogen bonds that link the molecules into zigzag chains.

Comment

Metal complexes based on Schiff bases have been extensively studied in biological, pharmacological, clinical and analytical applications due to their potential biological activities, such as antibacterial and antitumour properties (Kahwa *et al.* 1986). Consequently, a large number of metal complexes of Schiff bases have been prepared as mimics of active centres in various proteins and enzymes (Santos *et al.*, 2001). As part of our study, we have investigated the title compound, (I), used as a precursor in the preparation of Schiff bases.



(I)

In the title molecule (Fig. 1), bond lengths and angles are within their normal ranges (Allen *et al.*, 1987). The ethylvanillin group (C7–C12/C15/O3/O4) is nearly planar, with an r.m.s. deviation for the fitted atoms of 0.0315 Å. This group makes a dihedral angle of 43.97 (8)° with the phenyl ring (C1–C6).

Packing is stabilized by weak non-classical intermolecular C—H···O═C hydrogen bonds that link adjacent molecules into zigzag chains running along the *a* axis (Table 1, Fig. 2).

Experimental

An anhydrous benzene solution (100 ml) of 3-ethoxy-4-hydroxybenzaldehyde (1.66 g, 10 mmol) was added dropwise to a solution (100 ml) of benzenesulfonyl chloride (1.76 g, 10 mmol) and pyridine (1.58 g, 20 mmol) in benzene over a period of 30 min, and the mixture was then stirred at 343 K for 24 h under N_2. The solvent was removed and the resultant mixture poured into ice–water (100 ml). The white precipitate which formed was then isolated, recrystallized from acetonitrile and dried *in vacuo* to give the pure compound in 56% yield. Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{15}H_{14}O_5S$
M_r = 306.33
Orthorhombic, *Pbca*
a = 7.5538 (15) Å
b = 13.511 (3) Å
c = 28.994 (6) Å
V = 2959.1 (11) Å^3
Z = 8
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.18 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.928, T_{max} = 0.972
12380 measured reflections
2601 independent reflections
1556 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.118
S = 1.00
2601 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.9638P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O5^{i}	0.93	2.55	3.309 (4)	139

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

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

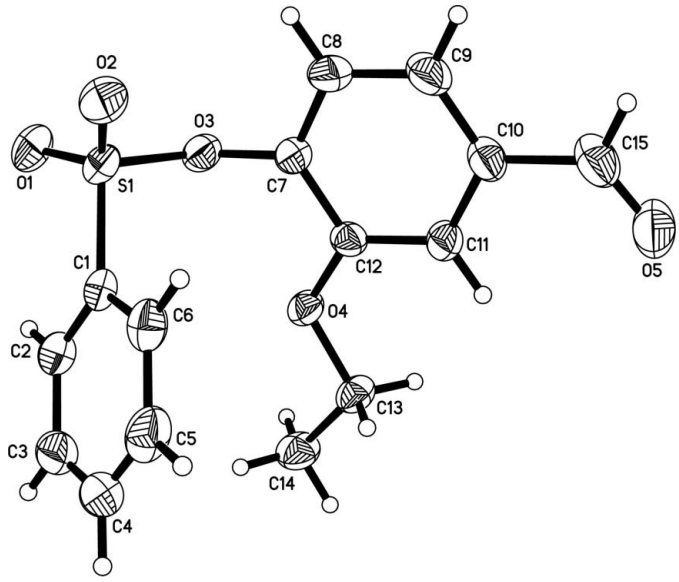


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

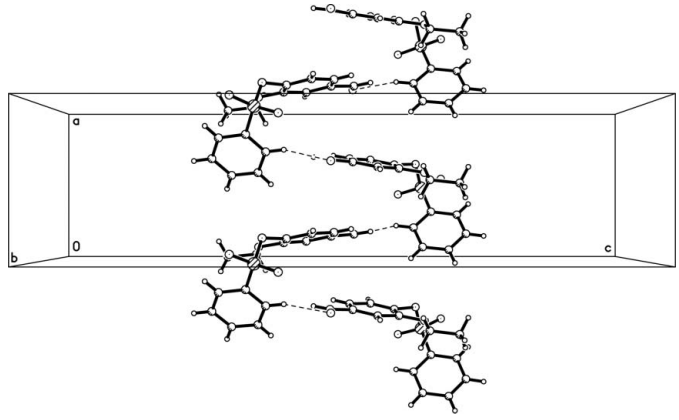


Figure 2
A partial packing diagram for (I), with hydrogen bonds drawn as dashed lines.

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