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4-Formyl-2-methoxyphenyl 4-methylbenzenesulfonate

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In the title compound, $C_{15}H_{14}O_5S$, the vanillin group makes a dihedral angle of 42.17 (12)° with the benzene ring. Packing is stabilized by weak non-classical intermolecular C—H···O hydrogen-bonding interactions, forming a two-dimensional network.

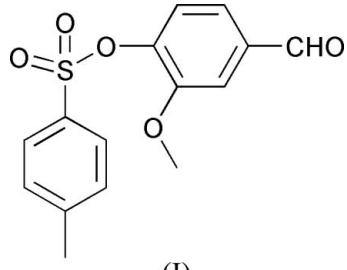
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.057
wR factor = 0.196
Data-to-parameter ratio = 13.1

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

Comment

Schiff base ligands have received a good deal of attention in biology and chemistry (Kahwa *et al.*, 1986; Klayman *et al.*, 1979). Many Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics (Santos *et al.*, 2001). As part of our interest in the coordination properties of Schiff bases functioning as ligands, we have investigated the title compound, (I), used as a precursor in the preparation of Schiff bases.



(I)

In the molecule of (I) (Fig. 1), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The vanillin group (C8–C13/C15/O3/O4) is essentially planar, with an r.m.s. deviation for fitted atoms of 0.0079 Å. This group makes a dihedral angle of 42.17 (12)° with the benzene ring (C1–C6).

Packing is stabilized by weak non-classical intermolecular C—H···O hydrogen-bonding interactions (Table 1), forming a two-dimensional network (Fig. 2).

Experimental

An anhydrous benzene solution (100 ml) of 4-hydroxy-3-methoxybenzaldehyde (1.52 g, 10 mmol) was added dropwise to a benzene solution (100 ml) of 4-methylbenzene-1-sulfonyl chloride (1.91 g, 10 mmol) and pyridine (0.79 g, 10 mmol) over a period of 30 min, and the mixture was refluxed for 24 h under a nitrogen atmosphere. The solvent was removed and the resulting mixture poured into ice–water (100 ml). The white precipitate which formed was then isolated, recrystallized from acetonitrile and dried in a vacuum to give the pure compound in 61% yield. Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{15}H_{14}O_5S$
$M_r = 306.33$
Triclinic, $P\overline{1}$
$a = 7.787$ (7) Å
$b = 8.750$ (7) Å
$c = 11.083$ (10) Å
$\alpha = 95.956$ (15)°
$\beta = 99.931$ (14)°
$\gamma = 102.640$ (13)°
$V = 717.9$ (11) Å^3
$Z = 2$
$D_x = 1.417$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.24$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.26 × 0.22 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.921$, $T_{max} = 0.962$
3658 measured reflections
2516 independent reflections
1792 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.196$
$S = 1.08$
2516 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.126P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···O1^{i}	0.96	2.53	3.362 (5)	145
C7—H7B···O5^{ii}	0.96	2.56	3.513 (6)	175

Symmetry codes: (i) $x, y+1, z$; (ii) $x, y, z+1$.

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, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl 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*.

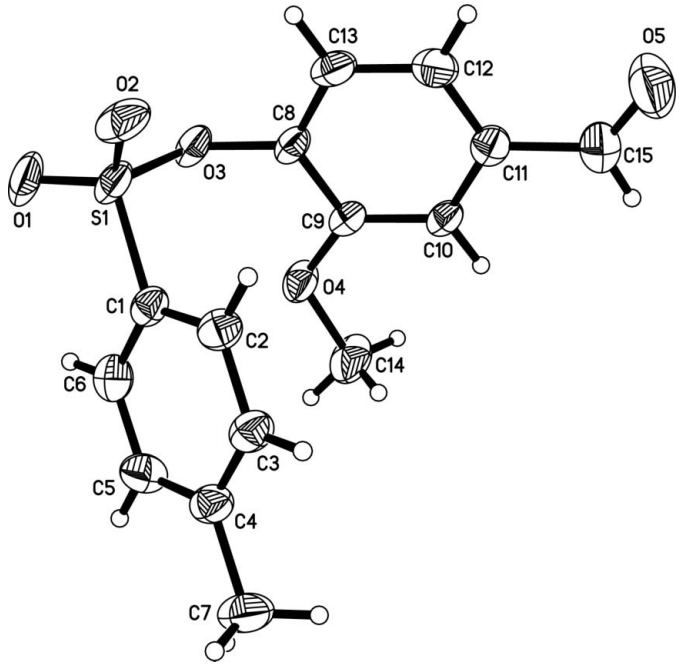


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

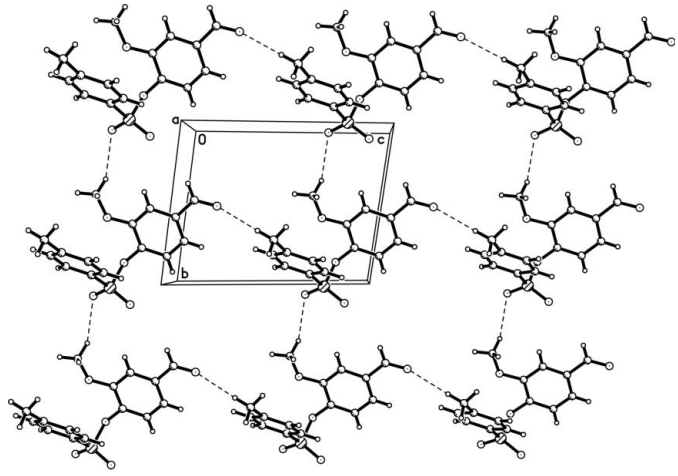


Figure 2
A packing diagram for (I), with hydrogen-bonding interactions drawn as dashed lines.

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