Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 5-Formyl-2-methoxyphenyl benzenesulfonate

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**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean σ(C–C) = 0.006 Å
*R* factor = 0.050
*wR* factor = 0.137
Data-to-parameter ratio = 12.9

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

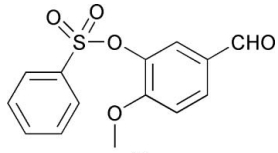


Received 31 October 2006
Accepted 16 November 2006

In the title compound, $C_{14}H_{12}O_5S$, the isovanillin group makes a dihedral angle of 37.45 (15)° with the phenyl ring. The crystal packing is stabilized by a weak non-classical intermolecular C—H···O hydrogen bond that links molecules into a chain.

## Comment

Schiff base ligands have received a good deal of attention in biology and chemistry (Kahwa *et al.*, 1986; Larson & Pecoraro, 1991). 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 (Zhang *et al.*, 2006), we report here the molecular structure of the title compound, (I), which is used as a precursor in the preparation of Schiff bases.




(I)

Bond lengths and angles in (I) (Fig. 1) are within normal ranges (Allen *et al.*, 1987). The isovanillin group (atoms C7–C13/O3/O4) is essentially planar, with an r.m.s. deviation for fitted atoms of 0.0075 Å. This group makes a dihedral angle of 37.45 (15)° with the phenyl ring (C1–C6). The crystal packing is stabilized by a weak non-classical intermolecular C—H···O═C hydrogen bond (Table 1) that links adjacent molecules into a chain running along the *c* axis (Fig. 2).

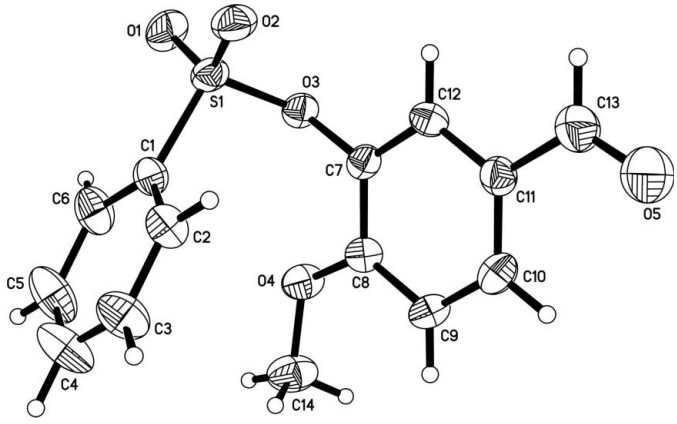



**Figure 1**
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

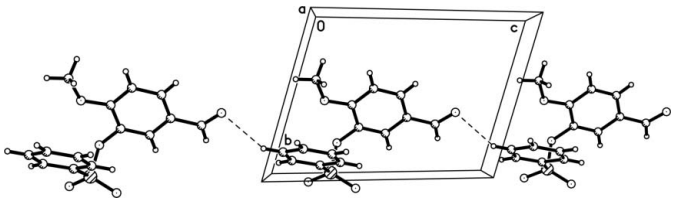



**Figure 2**
A partial packing diagram of (I), viewed along the *a* axis, with hydrogen bonds shown as dashed lines.

## Experimental

An anhydrous benzene solution (100 ml) of 3-hydroxy-4-methoxybenzaldehyde (1.52 g, 10 mmol) was added dropwise to a benzene solution (100 ml) of benzenesulfonyl chloride (1.76 g, 10 mmol) and pyridine (0.79 g, 10 mmol) and the mixture was refluxed for 24 h under nitrogen. The solvent was removed and the resultant mixture poured into ice–water (100 ml). The white precipitate was isolated, recrystallized from acetonitrile and then dried in a vacuum to give pure compound (I) in 58% yield. Colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

*Crystal data*

$C_{14}H_{12}O_5S$
$M_r$ = 292.31
Triclinic, $P\overline{1}$
$a$ = 7.915 (7) Å
$b$ = 8.255 (8) Å
$c$ = 11.581 (10) Å
$\alpha$ = 102.684 (14)°
$\beta$ = 109.208 (13)°
$\gamma$ = 97.137 (13)°
$V$ = 681.1 (11) Å$^3$
$Z$ = 2
$D_x$ = 1.425 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.25 mm$^{-1}$
$T$ = 294 (2) K
Block, colorless
0.28 × 0.26 × 0.16 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.918, $T_{max}$ = 0.960
3291 measured reflections
2365 independent reflections
1404 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041
$\theta_{max}$ = 25.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.137
$S$ = 1.01
2365 reflections
183 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.40 e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.064 (8)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C5—H5···O5$^{i}$ | 0.93 | 2.56 | 3.405 (6) | 151 |

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

H atoms were included in calculated positions (C—H = 0.93–0.96 Å) and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

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*.

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