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4-(2,4-Dichlorobenzyloxy)-3-ethoxybenzaldehyde

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.029
wR factor = 0.083
Data-to-parameter ratio = 8.4

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

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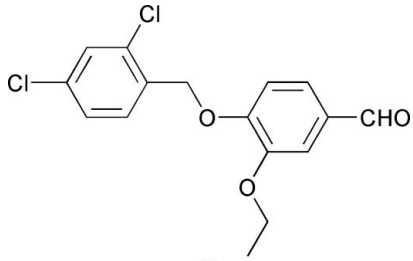
In the title compound, $C_{16}H_{14}Cl_2O_3$, the ethylvanillin group makes a dihedral angle of 6.15 (3)° with the dichlorobenzene ring. Intermolecular C—H···O interactions lead to trimeric associations of molecules.

Comment

As part of our ongoing studies (Zhen *et al.*, 2006) of the coordination properties of Schiff bases functioning as ligands, we have investigated the title compound, (I), which is used as a precursor in the preparation of Schiff bases.



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are within their normal ranges (Allen *et al.*, 1987). The ethylvanillin group (atoms C1–C6/C9/O1/O2) is essentially planar, with an r.m.s. deviation for the fitted atoms of 0.013 Å. Its mean plane makes a dihedral angle of 6.15 (3)° with the mean plane of the C11–C16 benzene ring.

The crystal structure of (I) is stabilized by weak intermolecular C—H···O interactions (Table 1 and Fig. 2), resulting in trimeric associations generated by a crystallographic threefold axis.

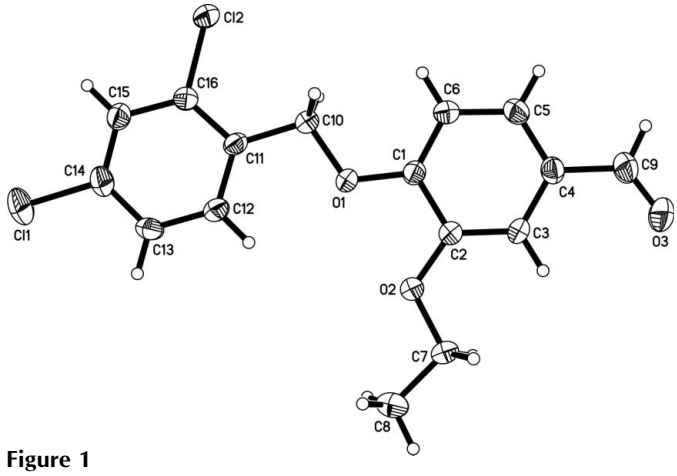


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

Experimental

An anhydrous acetonitrile solution (50 ml) of 3-ethoxy-4-hydroxybenzaldehyde (1.66 g, 10 mmol) was added dropwise to a solution (100 ml) of 1-(bromomethyl)-2,4-dichlorobenzene (2.40 g, 10 mmol) and potassium carbonate (1.38 g, 10 mmol) in acetonitrile over a period of 30 min, and the mixture refluxed for 24 h under a nitrogen atmosphere. The solvent was removed and the resultant mixture poured into ice–water (100 ml). The white precipitate was isolated and recrystallized from acetonitrile, and then dried in a vacuum to give the pure compound in 53% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{16}H_{14}Cl_2O_3$
M_r = 325.17
Trigonal, $R\overline{3}$
a = 19.849 (3) Å
c = 10.340 (2) Å
V = 3528.0 (10) Å^3
Z = 9
D_x = 1.378 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 294 (2) K
Block, colorless
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.878, T_{max} = 0.919
6567 measured reflections
1601 independent reflections
1263 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.083
S = 1.02
1601 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 0.7953P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3^{i}	0.93	2.52	3.429 (5)	167

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

Due to insignificant anomalous dispersion effects, Friedel pairs were merged before refinement. The molecule of (I) is achiral, thus any chirality in an individual crystal must arise from packing effects. The H atoms were included in calculated positions (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

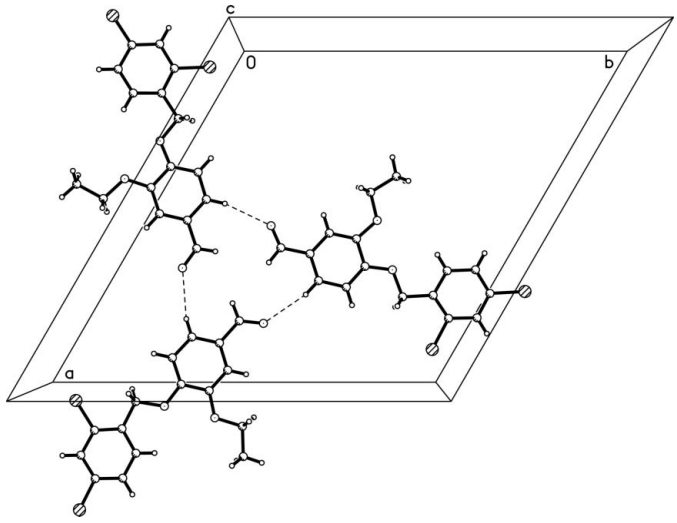


Figure 2
A trimeric association of molecules of (I), with C—H···O interactions swn as dashed lines.

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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