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4-(2,6-Dichlorophenyl)-1,4-dihydroxybutan-2-one

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Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.002 Å
R factor = 0.019
wR factor = 0.055
Data-to-parameter ratio = 15.2

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

Molecules of the title compound, $C_{10}H_{10}Cl_2O_3$, are linked by O—H···O hydrogen bonds into a sheet motif.

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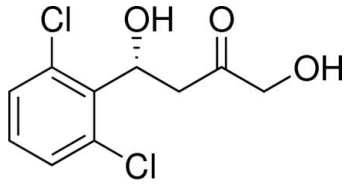
Comment

The title compound, (I), is an important reagent for the synthesis of 1,2,4-triols and substituted tetrahydrofurans (Chen *et al.*, 1987; Zheng *et al.*, 2005). It crystallizes as a monomeric molecule that interacts with adjacent molecules through hydrogen bonds (Table 1) to form a sheet motif. The carbonyl group is not involved in such interactions.



(I)

Experimental

To a solution of 2,6-dichlorobenzaldehyde (87.5 mg, 0.5 mmol) and (*S*)-*N*-phenylpyrrolidine-2-carboxamide (19 mg, 20 mmol) in a mixture of water (1 ml) and tetrahydrofuran (1 ml) was added hydroxyacetone (0.5 ml). The mixture was stirred at 273 K for 5 d. It was then treated with saturated ammonium chloride solution. The aqueous layer was extracted with ethyl acetate; the extract was dried over anhydrous magnesium sulfate. The solvent was removed and then purified by column chromatography on silica gel. Crystals were obtained by using ethanol as solvent.

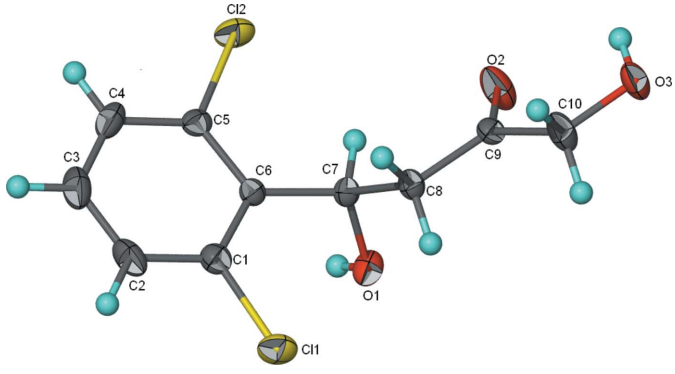


Figure 1
The molecular structure of (I) with 70% probability displacement ellipsoids (arbitrary spheres for H atoms).

Crystal data

$C_{10}H_{10}Cl_2O_3$
M_r = 249.08
Monoclinic, $P2_1$
a = 7.7674 (2) Å
b = 8.7852 (2) Å
c = 8.3555 (3) Å
β = 112.093 (1)°
V = 528.30 (3) Å^3
Z = 2
D_x = 1.566 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.60 mm^{-1}
T = 153 (2) K
Block, colorless
0.45 × 0.42 × 0.36 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.775, T_{max} = 0.814
5238 measured reflections
2205 independent reflections
2189 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.055
S = 1.08
2205 reflections
145 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 0.0574P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.145 (8)
Absolute structure: Flack (1983), 913 Friedel pairs
Flack parameter: 0.01 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···O3^{i}	0.85 (1)	2.02 (1)	2.844 (1)	164 (2)
O3—H3*O*···O1^{ii}	0.85 (1)	2.24 (2)	3.032 (2)	156 (2)

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

Carbon-bound H atom were positioned geometrically (C—H = 0.95–1.00 Å) and were allowed to ride on the parent C atoms, with U_{iso}(H) = 1.2U_{eq}(C). The hydroxy H atoms were located in a difference Fourier map and were refined with a distance restraint of O—H = 0.85 (1) Å; the displacement parameters were freely refined.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

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