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(2,4-Dichlorophenyl)methanol

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.027
wR factor = 0.074
Data-to-parameter ratio = 13.5

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

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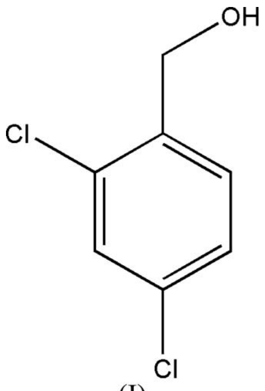
The title compound, $C_7H_6Cl_2O$, also known as 2,4-dichlorobenzyl alcohol, has antimicrobial properties and is widely used in pharmaceuticals. It crystallizes with two independent molecules in the asymmetric unit. The packing in the solid is characterized by the presence of ribbons of O—H···O hydrogen-bonded molecules, parallel to the *a* axis.

Comment

The title compound, 2,4-dichlorobenzyl alcohol, (I), was first introduced in the late 1950's as a fungicidal preservative in cosmetics and as an active ingredient in pharmaceuticals (Coogan *et al.*, 2004; Sundaraganesan *et al.*, 2006). It is widely employed as an antimicrobial agent in skin gels, creams, *etc.*, and its use in the Strepsils brand throat lozenge (Oxford *et al.*, 2005) is registered in many countries. Based on X-ray powder diffraction patterns, the lattice constants for the related, orthorhombic, 2,6-dichlorobenzyl alcohol, which also has antiseptic properties, have previously been reported (Roy *et al.*, 1993).



(I)

The crystal structure of (I) is monoclinic and contains two molecules in the asymmetric unit (Fig. 1). These have closely similar geometries, suggesting that the small, but consistent, deviations of their benzene rings from the idealized hexagonal geometry (Table 1) have electronic origin. Both molecules are planar, the largest deviations from the least-squares planes passing through all of the non-H atoms within each molecule being exhibited by C6 [0.050 (2) Å] and C10 [0.033 (2) Å]. There are zigzag arrangements of hydrogen-bonded molecules (Table 2), forming ribbons aligned with the crystallographic *a* axis (Fig. 2). These, in turn, are arranged in layers parallel to the *ab* cell face, their two-dimensional packing being apparently influenced by non-bonded interactions between the Cl atoms.

Experimental

Samples of (I) were kindly provided by SIMS (SIMS srl, Reggello Firenze, Italy). Crystals suitable for X-ray analysis were obtained by slow evaporation of a toluene/butanol (1:3 *v*/*v*) solution.

Crystal data

$C_7H_6Cl_2O$
$M_r = 177.02$
Monoclinic, $P2_1/c$
$a = 4.7361$ (4) Å
$b = 12.8179$ (13) Å
$c = 24.853$ (2) Å
$\beta = 96.852$ (8)°
$V = 1498.0$ (2) Å^3
$Z = 8$
$D_x = 1.570$ Mg m^{-3}
Cu *Kα* radiation
$\mu = 7.17$ mm^{-1}
$T = 296$ (2) K
Elongated prism, colorless
0.60 × 0.20 × 0.10 mm

Data collection

Oxford Diffraction Excalibur PX Ultra CCD diffractometer
ω scans
Absorption correction: multi-scan (*ABSPACK*; Oxford Diffraction, 2006)
$T_{\rm min} = 0.502$, $T_{\rm max} = 1.194$ (expected range = 0.205–0.488)
15434 measured reflections
2543 independent reflections
1967 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\rm max} = 64.9°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.074$
$S = 0.95$
2543 reflections
188 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 +]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.31$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C7—O1	1.415 (2)	C14—O2	1.415 (2)
C1—C7	1.512 (2)	C8—C14	1.514 (2)
C2—Cl1	1.7480 (17)	C9—Cl3	1.7487 (16)
C4—Cl2	1.7434 (17)	C11—Cl4	1.7432 (17)
C6—C1—C2	116.74 (15)	C13—C8—C9	116.91 (15)
C3—C2—C1	122.92 (16)	C10—C9—C8	122.92 (15)
C3—C4—C5	121.35 (16)	C12—C11—C10	121.58 (16)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.786 (17)	1.941 (17)	2.7228 (16)	173 (2)
O2—H2···O1$^{\rm i}$	0.789 (17)	1.929 (17)	2.7158 (16)	175 (2)

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

The crystal did not diffract very strongly and it was deemed that collecting data at θ higher than 64° would yield no improvement in the refinement. The O-bound H atoms were located in difference maps and their positions were refined with a unique O—H value and with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$. The other H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

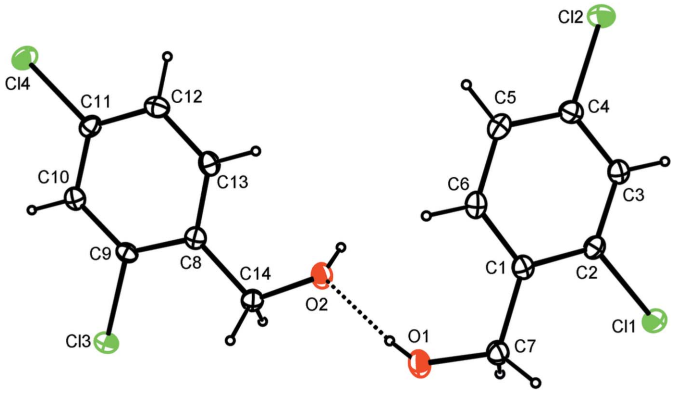


Figure 1
The asymmetric unit of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). The hydrogen bond is indicated by a dashed line.

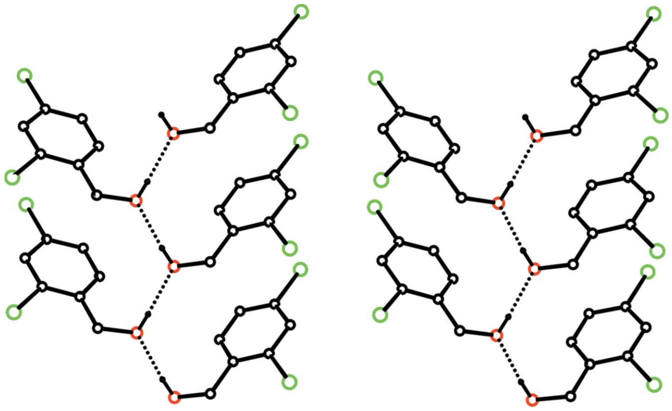


Figure 2
Part of the layer of molecules of (I) parallel to the *ab* cell face. H atoms not involved in hydrogen bonding (dashed lines) have been omitted.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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