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2-Hydroxymethyl-4-methylphenol

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The title compound, $C_8H_{10}O_2$, packs into a three-dimensional network *via* intermolecular O—H···O hydrogen-bonding interactions; a 12-membered ring is produced by hydrogen-bonded dimers.

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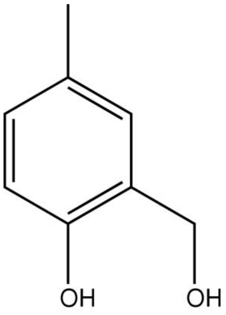
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.126
Data-to-parameter ratio = 15.9

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

Comment

Salicyl alcohol and its derivatives are very useful reactants in organic synthesis. Salicylaldehyde derivatives are commonly prepared directly by the oxidation of the corresponding salicyl alcohol. Furthermore, they are effectively used in medicine as a result of their physiological activities, such as anaesthetic, antispasmodic and antiseptic (Dunning *et al.*, 1936). Up until now, only a few structural determinations of related salicyl alcohols have been reported (Leger *et al.*, 1978; Zorkii *et al.*, 1985; Halit *et al.*, 1987; Cox, 2003).



(I)

The molecular structure of the title compound, (I), with the atom-numbering scheme is shown in Fig. 1, while selected bond distances and angles are given in Table 1. All the bond lengths and angles have normal values and are in good agreement with those found in similar compounds (Chu *et al.*, 2004, 2005). Apart from the O and H atoms of the hydroxymethyl group and the H atoms attached to C8, the whole molecule is essentially planar. The out-of-plane hydroxymethyl atom O2 is 1.317 (2) Å from the mean plane of the remaining non-H atoms in the molecule, the C2—C1—C7—O2 torsion angle being 72.7 (2)°.

All the O atoms in (I) contribute to the formation of intermolecular hydrogen bonds; however, no intramolecular hydrogen bonds are observed. Four O—H···O hydrogen bonds link every molecule with three neighbouring molecules, in which atoms O1 and O2 serve as both donors and acceptors. Thus, a 12-membered hydrogen-bonded ring (Fig. 2) is generated in each centrosymmetric dimer; this is similar to the situation in 4-bromo-2-hydroxymethylphenol (Cox, 2003).

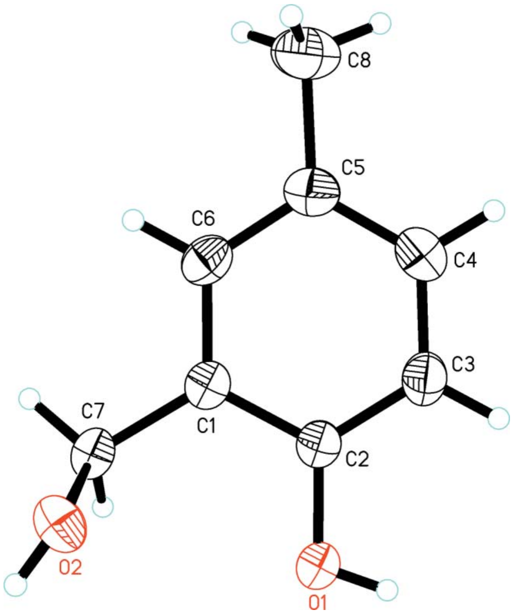


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

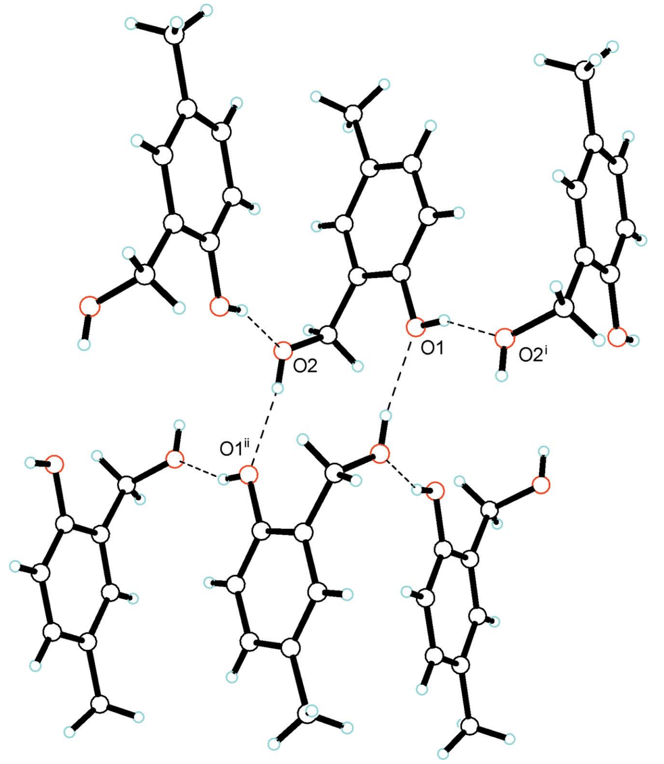


Figure 2
A perspective view of the intermolecular hydrogen-bond contacts in (I). Hydrogen bonds are shown as dashed lines. [Symmetry codes: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $1 - x, 1 - y, 2 - z$].

These O—H···O hydrogen-bond contacts help to form a three-dimensional network structure in (I) (Fig. 3). In the crystal packing, there are two sets of benzene rings, with a dihedral angle of 69.8 (2)°, and each set packs in a parallel fashion. Nevertheless, there is no evidence of significant π–π interactions due to the large offset between the two benzene rings. Inside these parallel rings, molecules are tightly associated into dimeric subunits around inversion centres by two complementary hydrogen bonds.

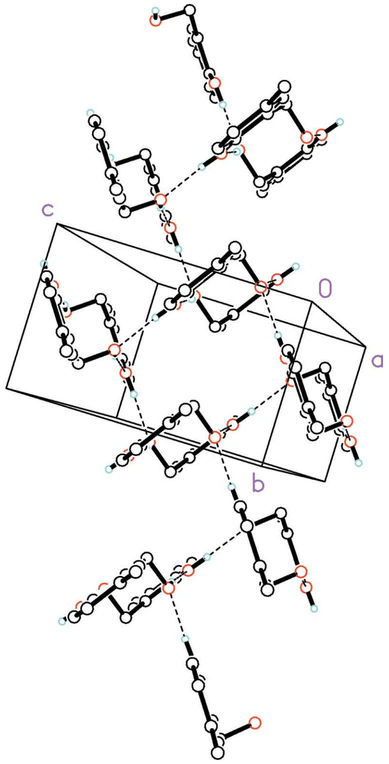


Figure 3
A three-dimensional packing diagram of (I). For clarity, only H atoms involved in hydrogen bonds are shown. Hydrogen-bond contacts are indicated by dashed lines.

Experimental

The title compound, (I), was prepared according to the literature method of Belyanin *et al.* (2001). Reaction of 4-methylphenol with paraformaldehyde in the presence of boric acid gave (I) in 73% yield [m.p. 377–378 K, literature 378–379 K (Nagata *et al.*, 1979)]. Elemental analysis calculated for $C_8H_{10}O_2$: C 69.54, H 7.30%; found: C 69.52, H 7.24%. Main FT–IR (KBr, cm^{-1}): 3437 (*s*), 3158 (*s*), 2963 (*s*), 2910 (*m*), 1619 (*m*), 1512 (*m*), 1485 (*m*), 1441 (*m*), 1411 (*m*), 1267 (*s*), 1124 (*s*), 1017 (*s*), 815 (*s*). ^{1}H NMR (CDCl$_3$, 298 K, TMS): 2.27 (*s*, 3H, CH$_3$), 4.85 (*s*, 2H, CH$_2$), 7.28 (*s*, 1H, OH), 7.04 (*s*, 1H, ArH), 7.02 (*s*, 1H, ArH), 6.87 (*s*, 1H, ArH), 6.80 (s, 1H, OH). Colourless single crystals of (I) suitable for X-ray analysis were grown from a toluene solution by slow evaporation at room temperature in air.

Crystal data

$C_8H_{10}O_2$
$M_r = 138.16$
Monoclinic, $P2_1/c$
$a = 16.322$ (3) Å
$b = 5.4697$ (9) Å
$c = 8.4504$ (14) Å
$\beta = 101.447$ (3)°
$V = 739.4$ (2) Å^3
$Z = 4$

$D_x = 1.241$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1038 reflections
$\theta = 2.5$–26.1°
$\mu = 0.09$ mm^{-1}
$T = 291$ (2) K
Block, colourless
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.985$, $T_{\max} = 0.994$
4132 measured reflections
1590 independent reflections
996 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.065$
$\theta_{\max} = 27.0^\circ$
$h = -11 \rightarrow 20$
$k = -6 \rightarrow 6$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.126$
$S = 0.92$
1590 reflections
100 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.14$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.494 (2)	C7—O2	1.4331 (18)
O2—C7—C1	109.21 (12)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2$^{\text{i}}$	0.82 (2)	1.89 (2)	2.670 (2)	158 (2)
O2—H2···O1$^{\text{ii}}$	0.86 (2)	1.96 (2)	2.805 (2)	169 (2)

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

The C-bound H atoms were placed in geometrically idealized positions (C—H = 0.93–0.97 Å) and refined as riding atoms, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl C atoms and $1.2U_{\text{eq}}(\text{C})$ for the methylene C atoms. The O-bound H atoms were located in a difference Fourier map and refined isotropically.

Data collection: *SMART* (Bruker 2000); cell refinement: *SAINT* (Bruker 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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