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(4-Hydroxy-2,5-dimethylphenyl)phenylmethanone

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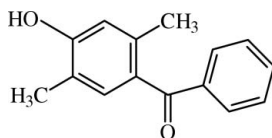
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Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.032; wR factor = 0.058; data-to-parameter ratio = 13.0.

The title compound, $\text{C}_{15}\text{H}_{14}\text{O}_2$, was obtained by Friedel–Crafts acylation between 2,5-dimethylphenol and benzoyl chloride in the presence of aluminium chloride as a catalyst. The dihedral angle between the benzene rings is $61.95(4)^\circ$. In the crystal, $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding and $\text{C}-\text{H}\cdots\text{O}$ weak interactions lead to polymeric $C(6)$, $C(8)$ and $C(11)$ chains along the a , b and c -axis directions, respectively.

Related literature

For background information on the anti-fungal and anti-inflammatory biological activity of benzophenones, see: Naldoni *et al.* (2009); Selvi *et al.* (2003); Naveen *et al.* (2006). For 104 benzophenone molecules, see: Cox *et al.* (2008). For hydrogen-bond motifs, see: Etter (1990).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{14}\text{O}_2$
 $M_r = 226.26$
 Orthorhombic, $Pbca$
 $a = 12.1392(10)$ Å
 $b = 8.1386(7)$ Å
 $c = 23.665(2)$ Å

$V = 2338.0(3)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 123$ K
 $0.25 \times 0.12 \times 0.05$ mm

Data collection

Oxford Diffraction Gemini S diffractometer
 Absorption correction: multi-scan (*CrysAlis CCD*; Oxford Diffraction, 2009)
 $T_{\min} = 0.904$, $T_{\max} = 1.000$

9067 measured reflections
 2059 independent reflections
 1061 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.058$
 $S = 0.73$
 2059 reflections

158 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.15$ e Å⁻³
 $\Delta\rho_{\min} = -0.14$ e Å⁻³

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2}\cdots\text{O1}^{\text{i}}$	0.84	1.92	2.6973 (15)	154
$\text{C15}-\text{H15B}\cdots\text{O1}^{\text{ii}}$	0.98	2.62	3.352 (2)	132
$\text{C4}-\text{H4}\cdots\text{O2}^{\text{iii}}$	0.95	2.67	3.454 (2)	140

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (ii) $-x + \frac{3}{2}, y - \frac{1}{2}, z$; (iii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PARST95* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2568).

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