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

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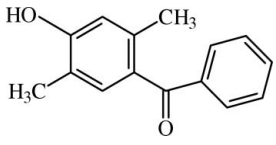
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.058; data-to-parameter ratio = 13.0.

The title compound, $C_{15}H_{14}O_2$, 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)°. In the crystal, O—H···O hydrogen bonding and C—H···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-inflamatory 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

$C_{15}H_{14}O_2$
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) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 123 K
0.25 × 0.12 × 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_{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···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.84	1.92	2.6973 (15)	154
C15—H15B···O1^{ii}	0.98	2.62	3.352 (2)	132
C4—H4···O2^{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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