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#### Key indicators

Single-crystal X-ray study  
 $T = 110$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.001$  Å  
 $R$  factor = 0.038  
 $wR$  factor = 0.108  
Data-to-parameter ratio = 20.2

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

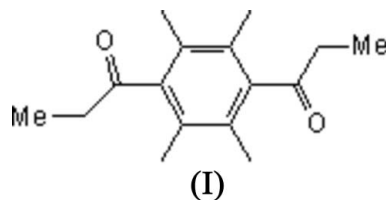
## Dipropiodurene

The conformer present in the crystal structure of the title compound [systematic name: 1,1'-(2,3,5,6-tetramethyl-*p*-phenylene)dipropan-1-one],  $\text{C}_{16}\text{H}_{22}\text{O}_2$ , lies on an inversion center and consequently has the two carbonyl groups in a *trans* orientation relative to the central ring. In the crystalline state, the planes of the carbonyl and attached methylene groups are at a dihedral angle of  $86.50(11)^\circ$  relative to the central ring.

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### Comment

In the present crystallographic study of the title compound, (I), the two carbonyl groups and attached methylene C atoms are in a *trans* orientation relative to the central ring (Fig. 1) due to the inversion center at the mid-point of the benzene ring. The planes of the carbonyl group and attached methylene C atom are at an angle of  $86.50(11)^\circ$  relative to the central ring. This can be compared with a crystallographic study of 1,4-bis(4-chlorobenzoyl)-2,3,5,6-tetramethylbenzene by Ferguson *et al.* (1993), who found that the two *p*-chlorobenzoyl groups were also in a *trans* orientation with a corresponding angle of  $85.9^\circ$ . A crystallographic study (Bear *et al.*, 1973) of a compound with a large pivaloyl group between two methyl groups (2,4,6-trimethyl-3-pivaloylbenzoic acid) reported the mean planes through the keto group and the benzene ring to have a dihedral angle of  $89.9^\circ$ . This compound was resolved but was found to undergo rapid racemization (Pinkus *et al.*, 1968). The corresponding angle for a related hindered duryl ester, ethyl 2,3,5,6-tetramethylbenzoate (Pinkus *et al.*, 2005), was found to be  $79.9^\circ$ .



Selected geometric parameters are presented in Table 1. All other bonds and angles are within expected ranges.

### Experimental

The title compound was prepared as follows. Anhydrous aluminium chloride (131 g, 1.2 mol), tetrachloroethane (500 ml), durene (26.8 g, 0.20 mol) and propionyl chloride (40.8 g, 0.44 mol) in a three-necked flask equipped with a reflux condenser were heated at 353 K for 16 h. The reaction mixture was decomposed by pouring into a cracked-ice/HCl mixture. The separated tetrachloroethane solution was washed with 10% sodium bicarbonate solution twice, followed by two

washings with water and final drying over anhydrous sodium sulfate. The solvent was removed by distillation and the product was recrystallized from benzene in 19% yield (9.3 g), m.p. 453.0–453.6 K [literature value 451 K (Baum & Meyer, 1895) 451 K]. Analysis calculated for  $C_{16}H_{22}O_2$ : C 78.01, H 9.00%; found (Galbraith Labs, Knoxville, Tennessee, USA): C 78.19, H, 9.07%. IR (dichloromethane):  $1703\text{ cm}^{-1}$  (C=O *str.*).

#### Crystal data

$C_{16}H_{22}O_2$	$Z = 4$
$M_r = 246.34$	$D_x = 1.174\text{ Mg m}^{-3}$
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
$a = 8.6268(14)\text{ \AA}$	$\mu = 0.08\text{ mm}^{-1}$
$b = 7.682(3)\text{ \AA}$	$T = 110(2)\text{ K}$
$c = 21.034(4)\text{ \AA}$	Block, colorless
$V = 1393.9(6)\text{ \AA}^3$	$0.30 \times 0.25 \times 0.21\text{ mm}$

#### Data collection

Bruker X8 APEX area-detector diffractometer	12799 measured reflections
$\varphi$ and $\omega$ scans	1715 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1535 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.974$ , $T_{\max} = 0.987$	$R_{\text{int}} = 0.034$
	$\theta_{\text{max}} = 28.2^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.3963P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.108$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.37\text{ e \AA}^{-3}$
1715 reflections	$\Delta\rho_{\text{min}} = -0.16\text{ e \AA}^{-3}$
85 parameters	
H-atom parameters constrained	

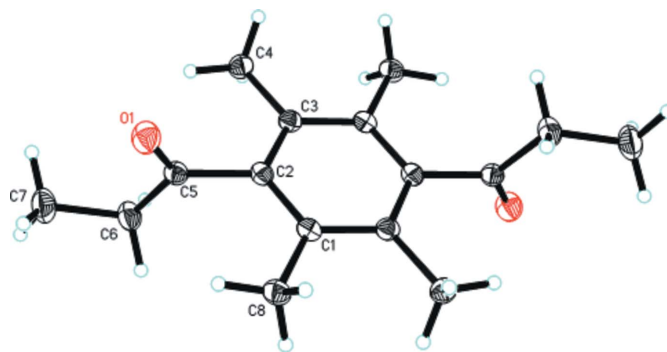
**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

C5–O1	1.2124 (13)	C5–C6	1.5101 (14)
C2–C5	1.5137 (12)		
C6–C5–C2	116.46 (8)		

All H atoms were included in calculated positions, with C–H = 0.98 and 0.99  $\text{\AA}$ , and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *APEX2* (Bruker, 2003); cell refinement: *APEX2*; data reduction: *SAINTE-Plus* (Bruker, 2003); program(s) used to solve



**Figure 1**

A view of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Unlabeled atoms are related to labeled atoms by the symmetry code  $(-x + 1, -y, -z + 1)$ .

structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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