

## 4'-Methylbiphenyl-2-carboxylic acid

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## Key indicators

Single-crystal X-ray study  
 $T = 173$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.032  
 $wR$  factor = 0.077  
Data-to-parameter ratio = 14.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $\text{C}_{14}\text{H}_{12}\text{O}_2$ , is used as an intermediate for the synthesis of various biologically active and pharmaceutical compounds. Bond lengths and angles adopt usual values. The dihedral angles between the two aromatic rings [ $53.39$  ( $3^\circ$ )] and between the carboxyl group and adjacent ring [ $42.37$  ( $10^\circ$ )] lie in the expected ranges. The crystal structure is characterized by centrosymmetric hydrogen-bonded dimers.

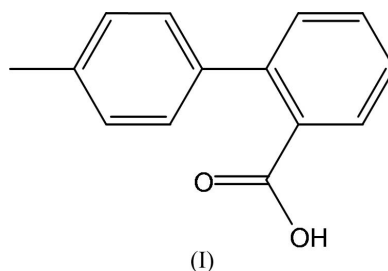
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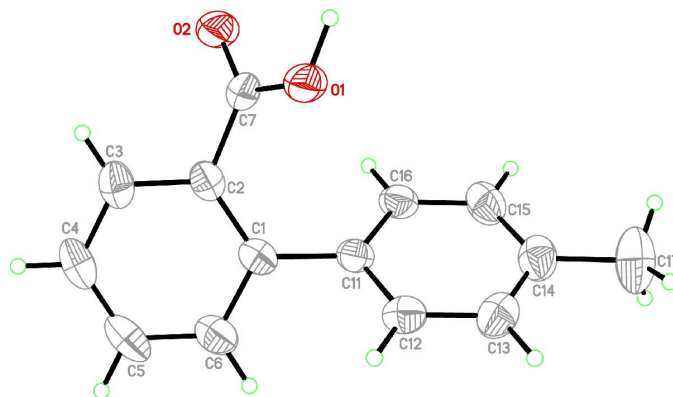
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## Comment

The title compound, (I), is used as an intermediate for the synthesis of various biologically active and pharmaceutical compounds (Gillis & Markham, 1997; Markham & Goa, 1997). In view of its importance and in order to determine the conformation of this molecule, a crystal structure determination has been carried out.



A perspective view of (I) is shown in Fig. 1. Bond lengths and angles (Table 1) can be regarded as normal [Cambridge Structural Database (CSD), Version 1.7; *MOGUL* Version 1.0.1; Allen, 2002]. The dihedral angle between the two



**Figure 1**  
Perspective view of the title compound, with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

aromatic rings is 53.39 (3)°. The carboxyl group subtends an angle of 42.37 (10)° with the ring to which it is attached. In seven comparable structures retrieved from the CSD containing the biphenyl-2-carboxylic acid moiety, the dihedral angles between the aromatic rings are in the range 44.9–62.9°, whereas the dihedral angles between the carboxyl group and the adjacent aromatic plane shows a significantly wider range of 32.5–85.9°. The molecules form hydrogen-bonded centrosymmetric dimers in the crystal structure (Table 2).

### Experimental

4'-Methylbiphenyl-2-carbonitrile (1.93 g, 10 mmol) was refluxed with methanol (10 ml) and 30% NaOH solution (10 ml) for 3 h to yield the title compound, which was recrystallized from dichloromethane (m.p. 419 K).

#### Crystal data

C <sub>14</sub> H <sub>12</sub> O <sub>2</sub>	$D_x = 1.199 \text{ Mg m}^{-3}$
$M_r = 212.24$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 8476 reflections
$a = 7.5953 (15) \text{ \AA}$	$\theta = 3.6\text{--}25.5^\circ$
$b = 14.582 (3) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 10.616 (2) \text{ \AA}$	$T = 173 (2) \text{ K}$
$\beta = 90.610 (16)^\circ$	Block, colourless
$V = 1175.7 (4) \text{ \AA}^3$	$0.30 \times 0.21 \times 0.11 \text{ mm}$
$Z = 4$	

#### Data collection

Stoe IPDS-II two-circle diffractometer	$R_{\text{int}} = 0.064$
$\omega$ scans	$\theta_{\text{max}} = 25.0^\circ$
5269 measured reflections	$h = -9 \rightarrow 9$
2073 independent reflections	$k = -17 \rightarrow 17$
1528 reflections with $I > 2\sigma(I)$	$l = -10 \rightarrow 12$

#### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$
$wR(F^2) = 0.077$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.88$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2073 reflections	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
147 parameters	$\Delta\rho_{\text{min}} = -0.11 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

C1–C11	1.5011 (18)	C7–O2	1.2287 (15)
C2–C7	1.4920 (17)	C7–O1	1.3225 (14)
O2–C7–O1	122.50 (10)	O1–C7–C2	115.78 (11)
O2–C7–C2	121.65 (10)		

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 $\cdots$ O2 <sup>i</sup>	0.84	1.83	2.6604 (13)	170

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

All H atoms were located in a difference map, but were then positioned geometrically and refined with fixed individual displacement parameters (set at 1.2 times  $U_{\text{eq}}$  of the parent atom, but  $1.5U_{\text{eq}}$  for hydroxyl and methyl groups) using a riding model, with O–H = 0.84 Å and C–H = 0.95 and 0.98 Å for aromatic and methyl H atoms, respectively. In addition, the torsion angles of the hydroxyl group and the methyl group were refined.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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