

4'-Methylbiphenyl-2-carboxylic acid

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Key indicators

Single-crystal X-ray study
 $T = 173\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.032
 wR factor = 0.077
 Data-to-parameter ratio = 14.1

For 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.

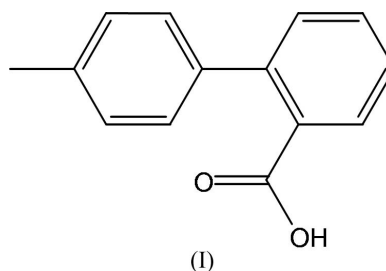
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Comment

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

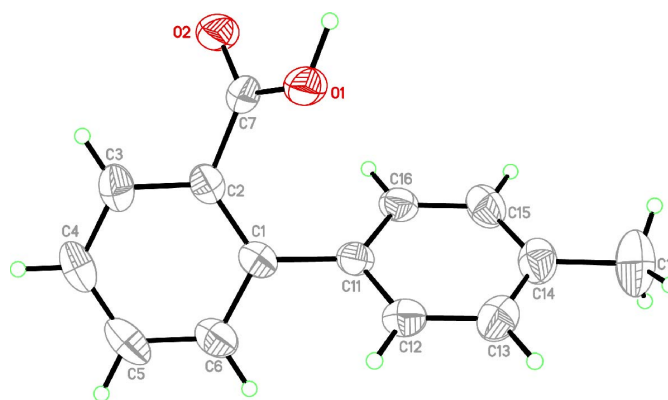


Figure 1

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

aromatic rings is $53.39(3)^\circ$. The carboxyl group subtends an angle of $42.37(10)^\circ$ 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 $44.9\text{--}62.9^\circ$, whereas the dihedral angles between the carboxyl group and the adjacent aromatic plane shows a significantly wider range of $32.5\text{--}85.9^\circ$. 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

$\text{C}_{14}\text{H}_{12}\text{O}_2$	$D_x = 1.199 \text{ Mg m}^{-3}$
$M_r = 212.24$	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	$R_{\text{int}} = 0.064$
ω 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 (\AA , $^\circ$).

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 (\AA , $^\circ$).

$D\text{—H}\cdots A$	$D\text{—H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
$\text{O1—H1}\cdots\text{O2}^i$	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_{eq} of the parent atom, but $1.5U_{\text{eq}}$ for hydroxyl and methyl groups) using a riding model, with $\text{O—H} = 0.84 \text{ \AA}$ and $\text{C—H} = 0.95$ and 0.98 \AA 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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