The molecular structure of the title acid, C\textsubscript{15}H\textsubscript{14}O\textsubscript{2}, exhibits a trans-planar arrangement of the aromatic rings. The carboxyl group is inclined at an angle of 6.4 (1)° with respect to the attached benzene ring. The classical hydrogen-bonded carboxylic acid dimers (O···O = 2.7 Å), characterized by an $R_2^2(8)$ pattern, predominantly stabilize the supramolecular assembly.

Comment

Benzoic acid was among the first organic crystal structures to be examined by the application of the X-ray crystallography (Bragg, 1921, 1922). Since then, numerous structures of benzoic acid and its derivatives have been reported (Sim et al., 1955; Parkin et al., 2005), owing to their importance in synthetic medicinal chemistry.

In the present report, we discuss the structure of one of these derivatives and the intermolecular interactions which govern its supramolecular assembly. The title acid, (I), is an intermediate in the preparation of dibenzosuberone (Ramesha & Roy, 2001) and the tricyclic antidepressant amitriptyline (Barbui et al., 2004; Maizels & McCarberg, 2005).
The molecule, shown in Fig. 1, assumes an overall trans conformation; \( \omega(C6-C7-C8-C9) = 175.8 (1)° \). The aromatic rings, linked by an ethylene bridge, are nearly parallel, with a dihedral angle of 4.3 (1)°. The plane of the carboxyl group is twisted by 6.4 (1)° out of the plane of the attached benzene ring (C9–C14).

The characteristic feature of the molecular packing is the formation of classical hydrogen-bonded carboxylic acid dimers (Fig. 2). The O2—H2A···O1 hydrogen-bond interaction involving centrosymmetrically related molecules is very strong (Table 1). The carboxylic acid dimers are characterized by an \( R(8) \) ring pattern (Bernstein et al., 1995). There are no significant overlaps of aromatic rings.

### Experimental

The title acid was obtained from Arvee Pharma Mysore, India. Crystals were grown by slow evaporation of an ethanol solution.

### Crystal data

\[
\begin{align*}
C_{15}H_{14}O_2 & \quad D_a = 1.227 \text{ Mg m}^{-3} \\
M_r & = 226.26 \\
Monoclinic, \ P2_1/c & \quad \text{Mo Kα radiation} \\
a = 13.7005 (2) \text{ Å} & \quad \text{Cell parameters from 1036} \\
b = 6.0509 (1) \text{ Å} & \quad \text{reflections} \\
c = 15.1789 (1) \text{ Å} & \quad \theta = 5–35° \\
\beta = 103.155 (1)° & \quad \mu = 0.08 \text{ mm}^{-1} \\
V = 1225.32 (3) \text{ Å}^3 & \quad T = 293 (2) \text{ K} \\
Z = 4 & \quad \text{Block, colorless} \\
\end{align*}
\]

### Data collection

1421 reflections with \( I > 2\sigma(I) \)

\[
\begin{align*}
\text{ Siemens SMART CCD area-detector diffractometer } & \quad R_{int} = 0.024 \\
\omega \text{ scans} & \quad \theta_{\text{max}} = 23.3° \\
\text{Absorption correction: none} & \quad h = -15 \rightarrow 14 \\
4864 measured reflections & \quad k = -6 \rightarrow 6 \\
1761 independent reflections & \quad l = -16 \rightarrow 14
\end{align*}
\]

### Refinement

\[
\begin{align*}
\text{Reefinement of } F^2 \quad R[F^2 > 2\sigma(F^2)] = 0.038 & \quad wR(F^2) = 0.114 \\
S = 1.08 & \quad w = 1/\sigma^2(F^2) + (0.0746P)^2 \\
1761 reflections & \quad (\Delta \sigma/\sigma)_{\text{max}} = 0.001 \\
159 parameters & \quad \Delta \rho_{\text{max}} = 0.18 \text{ e Å}^{-3} \\
& \quad \Delta \rho_{\text{min}} = -0.13 \text{ e Å}^{-3} \\
\text{Extinction correction: SHELXL97} & \quad \text{Extinction coefficient: 0.030 (4)}
\end{align*}
\]

### Table 1

<table>
<thead>
<tr>
<th>Hydrogen-bond geometry (Å, °)</th>
<th>D—H···A</th>
<th>D—H</th>
<th>H···A</th>
<th>D···A</th>
<th>D—H···A</th>
</tr>
</thead>
<tbody>
<tr>
<td>O2—H2A···O1</td>
<td>1.03 (2)</td>
<td>1.63 (2)</td>
<td>2.657 (2)</td>
<td>174 (2)</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry codes: (i) \(-x + 2, -y, -z + 2\).

All C-bound H atoms were positioned geometrically and refined as riding on their carrier atoms, with C—H = 0.93–0.97 Å and \( U_{eq}(H) = 1.2U_{eq}(\text{carrier atom}) \). The carboxylic H atom was located in a difference electron-density map and refined isotropically. The small crystal used in the analysis diffraeted rather poorly. The data set was limited to a maximum \( \theta \) angle of 23.3°, since only very weak diffraction was observed at higher angles.

Data collection: SMART (Siemens, 1995); cell refinement: SAINT (Siemens, 1995); data reduction: SAINT; program(s) used to solve structure: SHELXS86 (Sheldrick, 1985); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: WinGX (Farrugia, 1999) and PARST (Nardelli, 1995).

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### References


