The crystal structure of the title compound, C₈H₈O₄, is characterized by extensive hydrogen-bonding interactions to yield centrosymmetrically related dimers linked to each other by intermolecular interactions between the hydroxy groups and between the hydroxy and methyl groups.

Comment
The title compound, (I), was prepared as a prototype receptor with multiple functionality for coordination to analytes. The structure of (I) shows the molecules to be planar (Fig. 1), with bond lengths and angles in accord with conventional values (Allen et al., 1987). Pairs of centrosymmetrically related molecules are associated through bifurcated intra- and intermolecular hydrogen-bonding interactions between the α-hydroxy group and carbonyl O atoms to form a carboxylic acid dimer motif. Further hydrogen-bonding is observed between the 2- and 5-hydroxy groups on adjacent molecules (Fig. 2). In addition, the structure is stabilized through weak C–H · · · O hydrogen-bonding interactions between the ester methyl group and 5-hydroxy groups on adjacent molecules.
Data collection

Rigaku AFC-7R diffractometer
ω-2θ scans
Absorption correction: none
2012 measured reflections
1784 independent reflections
1353 reflections with I > 2σ(I)
Rint = 0.029

Refinement

Refinement on F²
R[F² > 2σ(F²)] = 0.044
wR(F²) = 0.140
S = 1.03
1784 reflections
110 parameters
H-atom parameters not refined

θmax = 27.5°
h = -7 → 15
k = 0 → 16
l = −6 → 6
3 standard reflections every 150 reflections
intensity decay: 0.5%

w = 1/[σ²(Fo²) + (0.092P)² + 0.1P]
where P = (Fo² + 2Fc²)/3
(Δσ)/max < 0.001
Δρmax = 0.23 e Å⁻³
Δρmin = -0.19 e Å⁻³

Extinction correction: SHELXL97
Extinction coefficient: 0.033 (9)

Table 1
Selected geometric parameters (Å, °).

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<tbody>
<tr>
<td>O21—C2</td>
<td>1.361 (2)</td>
<td>O72—C7</td>
</tr>
<tr>
<td>O51—C5</td>
<td>1.363 (2)</td>
<td>O72—C8</td>
</tr>
<tr>
<td>O71—C7</td>
<td>1.2133 (18)</td>
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<tr>
<td>C7—O72—C8</td>
<td>115.78 (12)</td>
<td>O51—C5—C6</td>
</tr>
<tr>
<td>O21—C2—C3</td>
<td>117.31 (13)</td>
<td>O72—C7—C1</td>
</tr>
<tr>
<td>O21—C2—C1</td>
<td>123.50 (13)</td>
<td>O71—C7—O72</td>
</tr>
<tr>
<td>O51—C5—C4</td>
<td>117.16 (13)</td>
<td>O71—C7—C1</td>
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</table>

Table 2
Hydrogen-bonding geometry (Å, °).

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<tbody>
<tr>
<td>O21—H21—O71</td>
<td>0.85</td>
<td>1.89</td>
<td>2.6205 (17)</td>
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<tr>
<td>O21—H21—O71i</td>
<td>0.85</td>
<td>2.43</td>
<td>3.0012 (18)</td>
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<tr>
<td>O51—H51—O21ii</td>
<td>0.85</td>
<td>1.92</td>
<td>2.7622 (17)</td>
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<tr>
<td>C8—H8B—O51iii</td>
<td>0.95</td>
<td>2.55</td>
<td>3.283 (2)</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) −x, 1−y, −z; (ii) 1/2±x, 3/2−y, 1/2±z; (iii) 1/2−x, y−1/2, 3/2−z.

H atoms were placed at calculated positions with C—H set to 0.95 Å. Hydroxy H atoms were located from a difference Fourier map and the O—H bond length set to 0.85 Å. Ueq values for the H atoms were set at 1.2Ueq of the parent atom.

Data collection: MSC/AFC-7 Diffractometer Control Software for Windows (Molecular Structure Corporation, 1999); cell refinement: MSC/AFC-7 Diffractometer Control Software for Windows; data reduction: TEXSAN for Windows (Molecular Structure Corporation, 1997–2001); program(s) used to solve structure: TEXSAN for Windows; program(s) used to refine structure: TEXSAN for Windows and SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: TEXSAN for Windows and PLATON (Spek, 1980–2001).

References


