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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.062
 wR factor = 0.181
Data-to-parameter ratio = 16.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

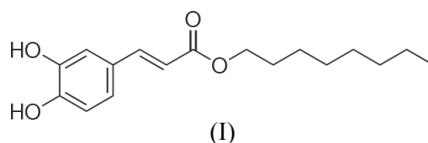
Octyl 3-(3,4-dihydroxyphenyl)prop-2-enoate

The title molecule, $\text{C}_{17}\text{H}_{24}\text{O}_4$, has an *E* configuration and shows normal values of bond lengths and angles. A bow angle was revealed in the longer ester group. The hydroxy groups contribute to intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, which link the molecules into ribbons extended in the $(\bar{1}10)$ direction.

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Comment

Caffeic acid and its derivatives are widely distributed in the plant kingdom (Chen *et al.*, 1999). These compounds exhibit anti-atherosclerotic, antibacterial, anti-inflammatory, anti-proliferative, immunostimulatory, anti-oxidative, antiviral and neuroprotective properties (Son & Lewis, 2002). In a continuation of our research on structure–activity relationships (Xia & Hu, 2005), we have obtained the title compound, (I), as a product of the modified Knoevenagel condensation reaction of 3,4-dihydroxybenzaldehyde and mono-octyl malonate.



The molecule of (I) has an *E* configuration; the carboxyl group and benzene ring are located on opposite sides of the $\text{C}7=\text{C}8$ bond (Fig. 1). All bond lengths and angles are in very close agreement with those found in similar caffeate structures (Xia *et al.*, 2004; Xia & Hu, 2005; Xia *et al.*, 2005, 2005*a,b*, 2006). The whole molecule is almost planar, with a mean deviation from the least-squares plane of 0.042 (2) Å, while atom C14 deviates from this plane by 0.133 (3) Å. Atoms C14–C17 form a plane, with a mean deviation of 0.009 (2) Å, and atom C13 deviates from this plane by 0.105 (6) Å. There is a bow angle of 7.12 (3)° at atom C13 of the ester group.

In the crystal structure, hydroxy groups contribute to intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1), which link the molecules into ribbons extended in the $(\bar{1}10)$ direction. Weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions (Table 1) are also observed in these ribbons. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

Experimental

Meldrum's acid (3.6 g, 25 mmol) was added to toluene (50 ml), and octanol (3.25 g, 25 mmol) was then added. The mixture was heated and refluxed for 5 h. When the mixture was cooled to room temperature, 3,4-dihydroxybenzaldehyde (1.4 g, 10 mmol), pyridine

(2.5 ml) and piperidine (0.25 ml) were added. The stirring continued at room temperature for 17 h. The solvents were distilled off *in vacuo*; the residue was dissolved in diethyl ether (30 ml), washed with a saturated solution of sodium bicarbonate (2×20 ml), diluted with hydrochloric acid (20 ml) and distilled water (20 ml). The diethyl ether was dried by anhydrous MgSO_4 overnight. After removal of the drier, the solvent was distilled off to give a yellow solid (2.6 g, 89%). Recrystallization from a mixture of acetone, diethyl ether and water (8:1:1) gave light-brown crystalline prisms (m.p. 405–406 K).

Crystal data

$\text{C}_{17}\text{H}_{24}\text{O}_4$	$V = 813.4 (6) \text{ \AA}^3$
$M_r = 292.36$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.194 \text{ Mg m}^{-3}$
$a = 5.454 (2) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 12.152 (5) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 12.584 (5) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\alpha = 87.763 (6)^\circ$	Prism, light brown
$\beta = 80.560 (6)^\circ$	$0.25 \times 0.20 \times 0.20 \text{ mm}$
$\gamma = 81.395 (5)^\circ$	

Data collection

Bruker APEX CCD area-detector diffractometer	3778 measured reflections
φ and ω scans	3137 independent reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	1607 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.969$, $T_{\max} = 0.983$	$R_{\text{int}} = 0.034$
	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0897P)^2]$
$wR(F^2) = 0.181$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3137 reflections	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
193 parameters	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2}\cdots\text{O1}$	0.82	2.26	2.711 (2)	115
$\text{O2}-\text{H2}\cdots\text{O1}^{\text{i}}$	0.82	2.20	2.914 (2)	146
$\text{O1}-\text{H1}\cdots\text{O3}^{\text{ii}}$	0.82	1.92	2.738 (2)	173
$\text{C2}-\text{H2A}\cdots\text{O3}^{\text{ii}}$	0.93	2.55	3.231 (3)	130

Symmetry codes: (i) $-x, -y + 2, -z$; (ii) $-x + 1, -y + 1, -z$.

The H atoms were placed in calculated positions ($\text{O}-\text{H} = 0.82 \text{ \AA}$ and $\text{C}-\text{H} = 0.93\text{--}0.97 \text{ \AA}$) and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{O,C})$.

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2003); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

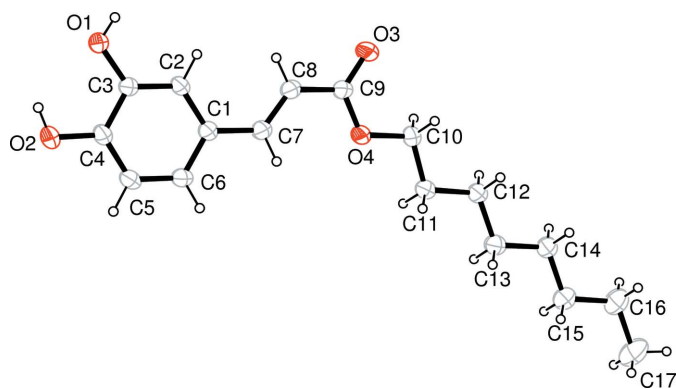


Figure 1
The structure of (I), shown with 30% probability displacement ellipsoids.

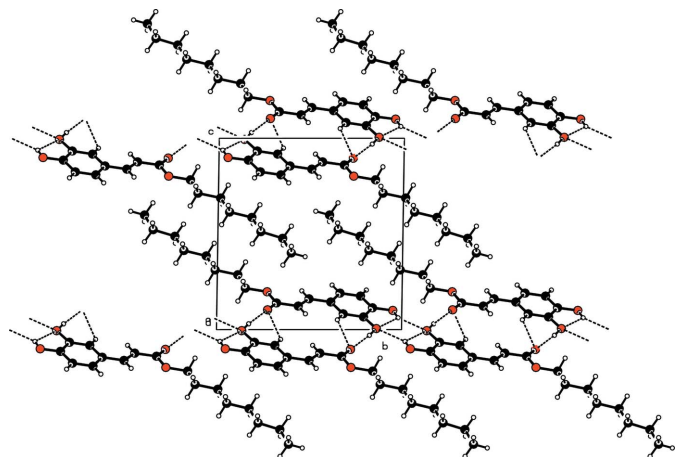


Figure 2
The packing diagram of (I), viewed along the a axis, showing the hydrogen bonds as dashed lines.

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