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(±)-2-Oxo-4-(2-oxo-2-phenylethyl)-5-phenyltetrahydrofuran-3-carboxylic acid

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.096
Data-to-parameter ratio = 17.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The stereochemistry about the lactone ring system of the title compound, $C_{19}H_{16}O_5$, has been established. Intermolecular hydrogen bonds are observed between carboxylic acid groups.

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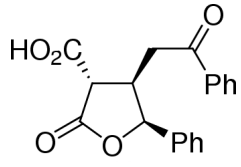
Comment

To establish the stereochemistry about the lactone ring system of (±)-ethyl 2-oxo-4-(2-oxo-2-phenylethyl)-5-phenyltetrahydrofuran-3-carboxylate (Greatrex *et al.*, 2002), the structure of the derived acid, (I), was determined. The molecular structure of (I) is shown in Fig. 1. A centrosymmetric dimer is formed through a strong intermolecular hydrogen bond between centrosymmetrically related carboxylic acid groups (Table 1).



(I)

Experimental

The title compound was prepared by base-catalysed hydrolysis of the parent ethyl ester, as previously described (Greatrex *et al.*, 2002). Crystals suitable for X-ray analysis were grown by slow evaporation from a CH_2Cl_2/hexane (1:1) solution of the compound.

Crystal data

$C_{19}H_{16}O_5$
M_r = 324.32
Monoclinic, $C2/c$
a = 30.0282 (4) Å
b = 8.9226 (1) Å
c = 12.1979 (2) Å
β = 104.884 (1)°
V = 3158.52 (8) Å^3
Z = 8
D_x = 1.364 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20303 reflections
θ = 3.4–28.3°
μ = 0.10 mm^{-1}
T = 123 (2) K
Prismatic, colourless
0.27 × 0.13 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Thick slice scans
21591 measured reflections
3871 independent reflections
3023 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 28.3°
$h = -40 \rightarrow 40$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 15$

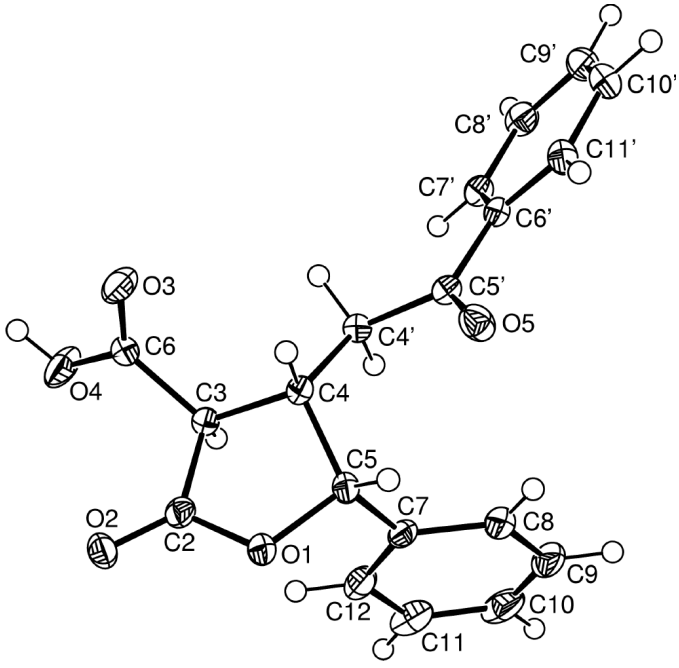


Figure 1
View of (I) (50% probability displacement ellipsoids).

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 2.4814P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.096$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
3871 reflections	
218 parameters	
H-atom parameters constrained	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3^{i}	0.84	1.84	2.6782 (14)	178

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

The H atoms were included in the riding-model approximation.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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