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(2*R*,3*S*)-Diethyl 2,3-dibenzoylsuccinate

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In the crystal structure of the title compound, $C_{22}H_{22}O_6$, the asymmetric unit consists of one half-molecule with the other half generated by a centre of inversion. The crystal packing is stabilized by C—H···O intermolecular interactions.

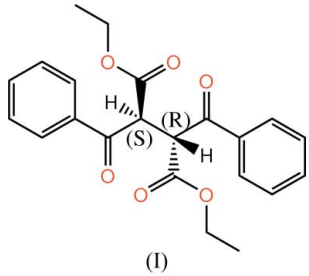
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.068
wR factor = 0.219
Data-to-parameter ratio = 13.4

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

Comment

1,4-Diketones are important intermediates for the synthesis of some natural products consisting of cyclopentanone and furan ring systems (McMurry & Meiton, 1971; Ito *et al.*, 1975, 1977). As part of a study of these compounds, we report the crystal structure of (2*R*,3*S*)-2,3-dibenzoylsuccinic acid diethyl ester, (I). The two aromatic rings are parallel (Fig. 1), the ethyl groups have a disordered methyl group and the crystal packing is stabilized by C—H···O intermolecular interactions as detailed in Table 1.



(I)

Experimental

The title compound was synthesized according to the literature procedure of Wu *et al.* (1997). Crystals appropriate for data collection were obtained by slow evaporation of a methanol–ethyl acetate (1:1 *v*/*v*) solution of (I).

Crystal data

$C_{22}H_{22}O_6$
M_r = 382.40
Monoclinic, $C2/c$
a = 11.328 (4) Å
b = 11.228 (4) Å
c = 15.986 (6) Å
β = 92.868 (6)°
V = 2030.7 (12) Å^3
Z = 4
D_x = 1.251 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 292 (2) K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
5177 measured reflections
1785 independent reflections
1095 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 25.0°

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.116P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.219$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
1785 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
133 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{ii}	0.93	2.59	3.388 (4)	145

Symmetry code: (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

The methyl group was found to be disordered over two orientations. The occupancies of the disordered positions C11/C11′ (and C11a/C11′a) refined to 0.540 (12)/0.460 (12). Suitable restraints were applied to the C—C distances involving the disordered atoms. The methyl H atoms were constrained to an ideal geometry with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93–0.98 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2003); software used to prepare material for publication: *SHELXTL*.

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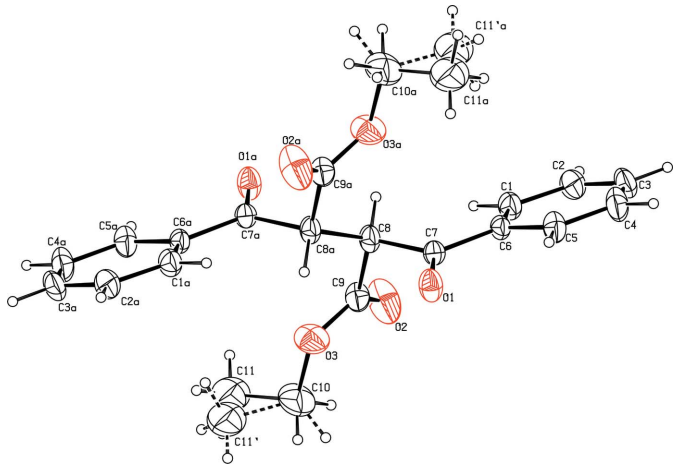

Figure 1
View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms labelled with the suffix a are related by ($-x$ + 1, $-y$ + 2, $-z$ + 1). Both disordered methyl components of the ethyl group are shown.

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