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Ethyl 2-(benzoyloxy)benzoate

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In the molecule of the title compound, $C_{16}H_{14}O_4$, the ester group is oriented with respect to the aromatic rings at dihedral angles of 7.74 (5) and 17.83 (4)°.

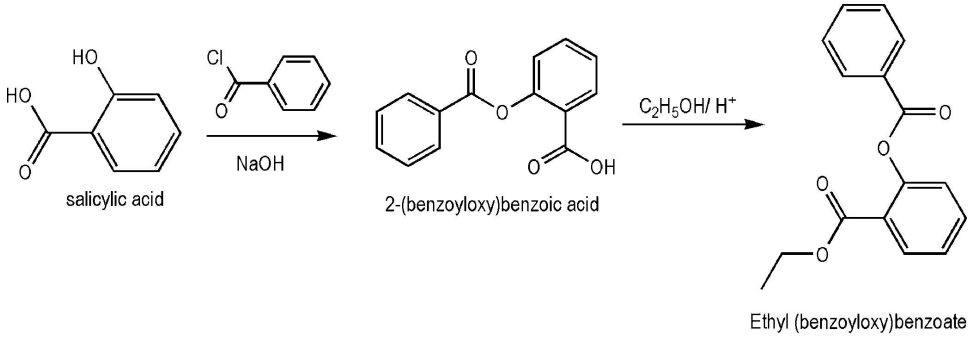
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.152
wR factor = 0.270
Data-to-parameter ratio = 13.2

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

Comment

The title compound, (I), is an intermediate in the synthesis of salicylic acid hydrazide. The crystal structure determination of (I), has been carried out in order to elucidate the molecular conformation. We report here the crystal structure of (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

Rings *A* (C1–C6) and *B* (C8–C13) are, of course, planar and the dihedral angle between them is 12.17 (4)°. The ester group (O3/C14–C16) is also planar, and is oriented at dihedral angles of 7.74 (5) and 17.83 (4)°, respectively, with respect to rings *A* and *B*.

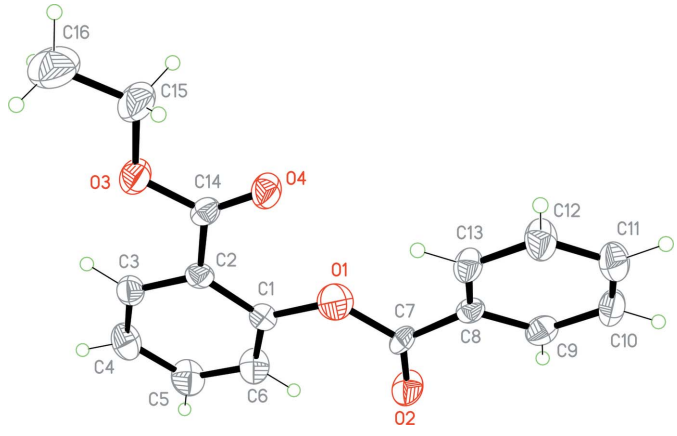


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

The title compound, (I), was synthesized in two steps by a literature method (Vogel, 1978). Benzoyl chloride (3.00 g, 22 mmol) was added dropwise to a stirred mixture of aqueous sodium hydroxide (10%) and salicylic acid (2.75 g, 20 mmol). The solid thus obtained was filtered, washed with water and recrystallized from aqueous ethanol (30%). The resulting protected salicylic acid (2.80 g, 20 mmol), absolute ethanol (80 ml) and concentrated sulfuric acid (0.7 ml) were refluxed for 6 h. The excess solvent was distilled off and the residue was filtered, washed with water and recrystallized from aqueous ethanol (40%), giving the pure title compound (I) (yield: 2.3 g, 84%; m.p. 382–384 K). Single crystals suitable for X-ray analysis were grown in ethanol by slow evaporation at room temperature.

Crystal data

$C_{16}H_{14}O_4$
$M_r = 270.27$
Monoclinic, $P2_1/c$
$a = 7.2123\ (12)$ Å
$b = 10.4116\ (17)$ Å
$c = 18.331\ (3)$ Å
$\beta = 98.259\ (4)^\circ$
$V = 1362.2\ (4)$ Å^3
$Z = 4$
$D_x = 1.318$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 298\ (2)$ K
Prism, colorless
$0.27 \times 0.18 \times 0.09$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.972$, $T_{max} = 0.990$
6982 measured reflections
2400 independent reflections
1808 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.152$
$wR(F^2) = 0.270$
$S = 1.32$
2400 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 3.0619P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O)$, where $x = 1.5$ for methyl and $x = 1.2$ for all other H atoms.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2002). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Vogel, A. I. (1978). *Vogel's Textbook of Practical Organic Chemistry, 4th* ed., edited by B. S. Furniss, A. J. Hannaford, V. Rogers, P. W. G. Smith and A. R. Tatchell, pp. 842–844. London: Longmann.