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Methyl 5-bromosalicylate

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.099
Data-to-parameter ratio = 16.2

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

In the title compound, $C_8H_7BrO_3$, an intramolecular hydrogen bond exists between the hydroxyl group and the O atom of the carbonyl group. The molecules are stacked along the b axis with weak π–π interactions.

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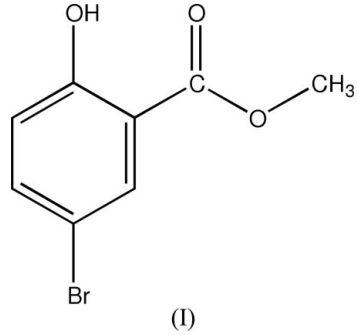
Comment

Salicylate compounds display a broad range of biological activities (Yuan & Tsao, 1994) and useful properties (Liu *et al.*, 1996). As part of our ongoing studies (Jin & Xiao, 2005; Jin *et al.*, 2004) on activated esters and their complexes, the preparation and X-ray crystal structure determination of the title compound, (I), was undertaken. Bond lengths and angles in (I) show normal values (Jin & Xiao, 2005; Table 1). The non-H atoms of the molecule lie in a plane, with an r.m.s deviation of 0.009 Å. An intramolecular hydrogen bond is observed between the hydroxyl group and the O atom of the carbonyl group (Fig. 1 and Table 2). The molecules translated one unit cell along the b-axis direction are stacked with C1···C7^{i} and C6···C7^{i} [symmetry code (i): x, 1 + y, z] distances of 3.562 (4) Å and 3.599 (4) Å, respectively, indicating weak π-π interactions.



(I)

Experimental

Compound (I) was synthesized according to the literature procedure of Bartlett & Trachtenberg (1958). Single crystals suitable for X-ray diffraction were grown by slow evaporation of a methanol solution at room temperature.

Crystal data

$C_8H_7BrO_3$
M_r = 231.05
Monoclinic, $C2/c$
a = 29.203 (7) Å
b = 4.0724 (10) Å
c = 16.679 (4) Å
β = 120.465 (3)°
V = 1709.7 (7) Å^3
Z = 8
D_x = 1.795 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2046 reflections
θ = 2.5–27.1°
μ = 4.77 mm^{-1}
T = 273 (2) K
Block, colourless
0.65 × 0.40 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.123, T_{max} = 0.350
4772 measured reflections
1849 independent reflections
1511 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.0°
$h = -36 \rightarrow 34$
$k = -4 \rightarrow 5$
$l = -21 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.06
1849 reflections
114 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.561P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C5	1.890 (3)	C7—O2	1.213 (4)
C1—C7	1.479 (4)	C7—O3	1.328 (4)
C2—O1	1.351 (4)	C8—O3	1.449 (4)
O1—C2—C3	117.5 (3)	O2—C7—C1	123.7 (3)
O1—C2—C1	122.9 (3)	C7—O3—C8	116.2 (3)
O2—C7—O3	123.6 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.93 (4)	1.78 (4)	2.617 (4)	149 (4)

The hydroxyl H atom was located in a difference Fourier map and refined isotropically [O—H = 0.93 (4) Å]. All other H atoms were included in the riding-model approximation, with C—H distances of 0.93 Å (aromatic H atoms) and 0.96 Å (methyl atoms). The isotropic displacement parameters were set equal to $1.2U_{eq}$ of the carrier atom for the aromatic and to $1.5U_{eq}$ of the carrier for methyl H atoms.

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, 2001); software used to prepare material for publication: *SHELXTL*.

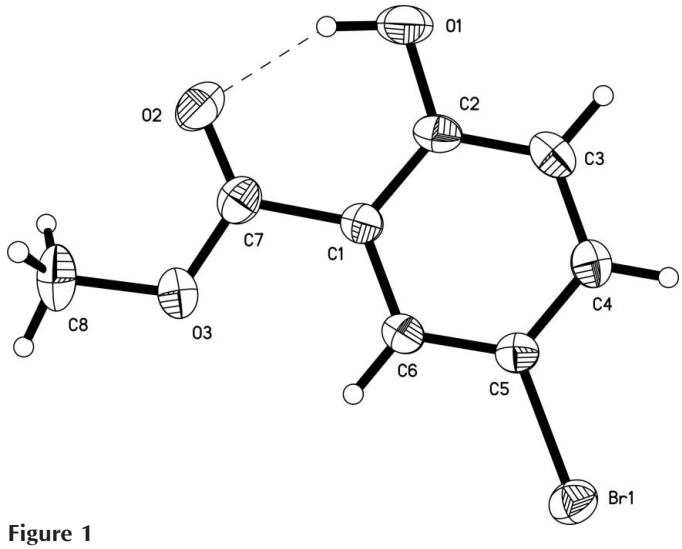


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

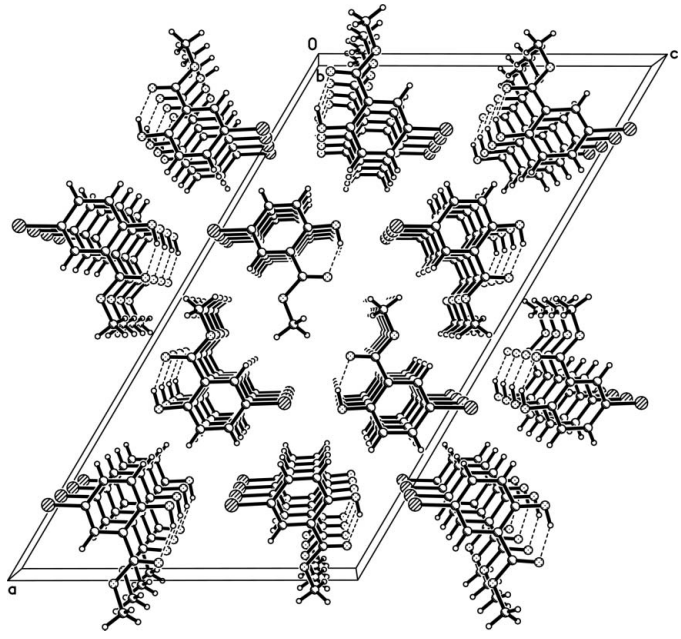


Figure 2
Packing diagram for (I). Hydrogen bonds are indicated by dashed lines.

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