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(3-Methylsulfanyl-2-phenyl-1-benzofuran-5-yl)-acetic acid

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Key indicators

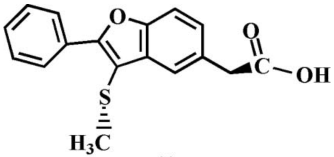
Single-crystal X-ray study
T = 173 K
Mean *σ*(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.120
Data-to-parameter ratio = 16.0

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

The title compound, $C_{17}H_{14}O_3S$, was prepared by the Lewis acid-catalysed reaction of 4-hydroxyphenylacetic acid with 2-chloro-2-(methylsulfanyl)acetophenone. The 1-benzofuran ring system is nearly planar. The crystal structure is stabilized by aromatic π–π stacking interactions and inversion-related intermolecular O—H$\cdots$O hydrogen bonds between the carboxyl groups.

Comment

This work follows from our previous report on [2-methyl-3-methylsulfanyl-1-(benzofuran-5-yl)]acetic acid (Choi *et al.*, 2006). The isomeric title compound, (I) (Fig. 1), was obtained by the one-pot reaction of 4-hydroxyphenylacetic acid with 2-chloro-2-(methylsulfanyl)acetophenone in the presence of zinc chloride.



(I)

In (I), bond lengths and angles are as expected for this type of compound (Choi *et al.*, 2006) and the 1-benzofuran unit is almost planar, with a mean deviation of 0.005 Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle between the phenyl ring and the benzofuran unit is 2.5 (1)°; the carboxyl group and the methyl group of the methylsulfanyl substituent lie on opposite sides of the plane of the benzofuran unit.

In the crystal structure (Fig. 2), π–π stacking interactions occur between the 2-phenyl group and the furan ring of the benzofuran system with $Cg1\cdots Cg2^{i}$ = 3.666 (4) Å [*Cg*1 is the centroid of the C9—C14 ring and *Cg*2 is the centroid of the C1—C3/C8/O1 ring; symmetry code: (i) $1 + x, y, z$], and between the furan and benzene rings of adjacent benzofuran systems, with $Cg2\cdots Cg3^{i}$ = 3.887 (4) Å [*Cg*3 is the centroid of the C3–C8 ring]. Classical inversion-related $O3–H3\cdots O2^{ii}$ hydrogen bonds [Symmetry code: (ii) $-1 - x, 2 - y, -z$] link carboxyl groups of adjacent molecules (Table 1, Fig. 2).

Experimental

The title compound, (I), was prepared by a procedure previously established for substituted benzo[*b*]furans (Choi *et al.*, 1998). Zinc chloride (354 mg, 2.6 mmol) was added at room temperature to a stirred solution of 2-chloro-2-(methylsulfanyl)acetophenone (521 mg, 2.6 mmol) and 4-hydroxyphenylacetic acid (396 mg, 2.6 mmol) in dichloromethane (30 ml) and tetrahydrofuran (3 ml). The mixture was stirred for 40 min and quenched with water. The organic layer was separated, dried over magnesium sulfate, filtered and concentrated under vacuum. The residue was purified by column chromatography (hexane–EtOAc 1:1) to afford (I) as a colorless solid. Crystals suitable for *X*-ray analysis were grown by slow evaporation of an acetone solution [yield 44%, m.p. 471–473 K; $R_f = 0.48$ (hexane–EtOAc 1:1)].

Crystal data

$C_{17}H_{14}O_3S$
$M_r = 298.34$
Monoclinic, $P2_1/c$
$a = 5.1605$ (4) Å
$b = 15.585$ (1) Å
$c = 17.570$ (1) Å
$\beta = 95.085$ (1)°
$V = 1407.53$ (16) Å^3

$Z = 4$
$D_x = 1.408$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.24$ mm^{-1}
$T = 173$ (2) K
Block, colorless
0.64 × 0.25 × 0.25 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: none
8427 measured reflections

3039 independent reflections
2763 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.038$
$\theta_{\rm max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.120$
$S = 1.23$
3039 reflections
190 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 1.3997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.32$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.31$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2$^{\rm ii}$	0.82	1.83	2.639 (2)	169

Symmetry code: (ii) $-x-1, -y+2, -z$.

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for aromatic H atoms, 0.96 Å, $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl H atoms, and O—H = 0.82 Å, $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

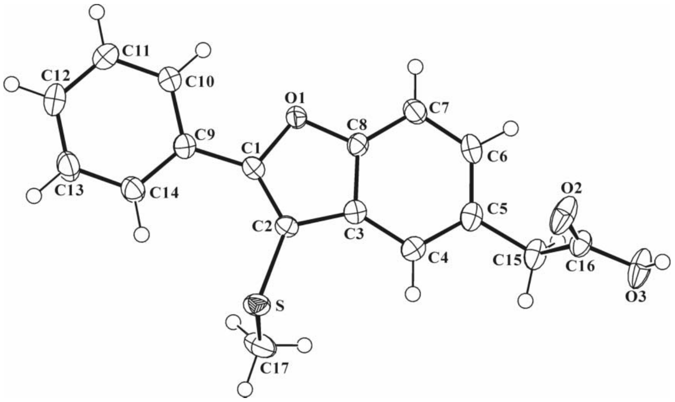


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

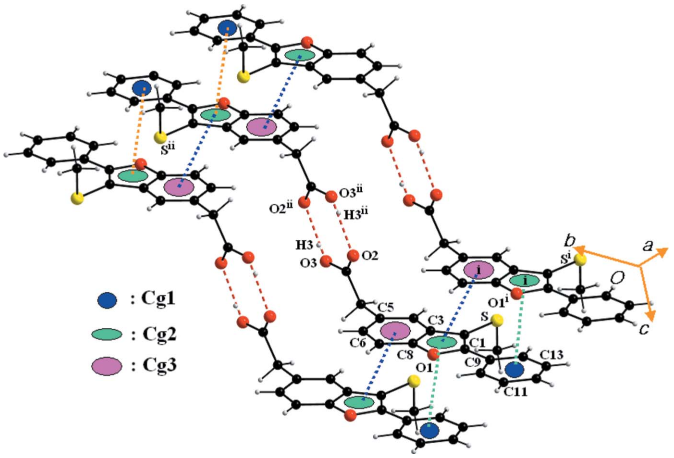


Figure 2
$\pi\cdots\pi$ Interactions (dashed lines) in (I). *Cg* denotes the centroid of a ring. [Symmetry codes: (i) $1 + x, y, z$; (ii) $-1 - x, 2 - y, -z$.]

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