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2-(2-Methoxyphenylsulfanyl)benzoic acid

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Key indicators

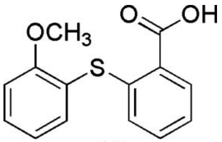
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.056
wR factor = 0.162
Data-to-parameter ratio = 12.9

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

The title compound, $C_{14}H_{12}O_3S$, was synthesized from 2-methoxythiophenol and 2-chlorobenzoic acid with copper powder as catalyst. In the molecule, the two benzene ring planes are roughly perpendicular. The molecules are linked through an inversion center by O—H⋯O hydrogen bonds, forming a pseudo-dimer.

Comment

Substituted diphenyl sulfide derivatives are a class of compounds which display high *in vitro* and *in vivo* affinities for serotonin transporter (SERT), high selectivity for dopamine transporter sites (DAT) and partial selectivity over norepinephrine transporter sites (NET), and have been described as potent and selective SERT ligands (Wilson *et al.*, 2000).



(I)

The molecular structure of the title compound, (I), is illustrated in Fig. 1. In the molecule, the two benzene rings make a dihedral angle of 78.50 (12)°. The most interesting feature is the occurrence of O—H⋯O hydrogen bonding linking two molecules through an inversion center to form a pseudo-dimer (Table 1 and Fig. 2).

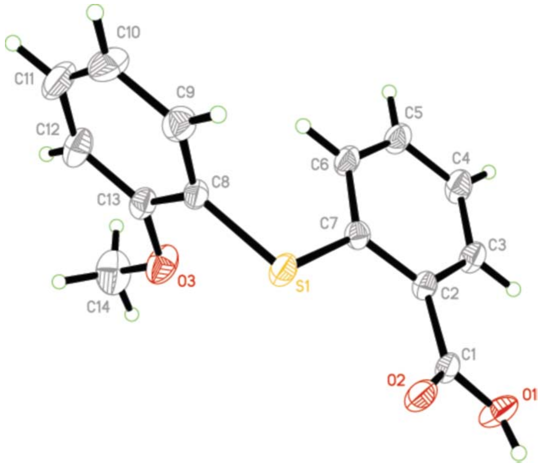


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

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Experimental

A mixture of 2-methoxythiophenol (6.72 g, 48 mmol), 2-chlorobenzoic acid (6.26 g, 40 mmol), K_2CO_3 (19.9 g, 144 mmol), and copper powder (0.8 g, 12.6 mmol) in dimethylformamide (120 ml) was stirred at 373 K for 24 h. After cooling and dilution with water (600 ml), the mixture was filtered through diatomaceous earth and the filtrate was acidified to pH 7.0 with aqueous HCl (6 mol l^{-1}). After filtration, the filtrate was acidified to pH 3.0 again with aqueous HCl(6 mol l^{-1}) and cooled. The white precipitate was collected by filtration and washed with water, then dried to yield the title compound as a white powder (Mehta & Brieaddy, 1997; Wilson & Houle, 1999; Younes *et al.*, 2000; Wilson *et al.*, 2000). Crystals suitable for X-ray analysis were grown by slow evaporation of an absolute methanol solution at room temperature over a period of 15 d.

Crystal data

$C_{14}H_{12}O_3S$
M_r = 260.30
Triclinic, $P\overline{1}$
a = 7.165 (3) Å
b = 7.768 (3) Å
c = 11.907 (4) Å
α = 103.505 (6)°
β = 100.886 (6)°
γ = 101.474 (6)°
V = 612.0 (4) Å^3
Z = 2
D_x = 1.413 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1160 reflections
θ = 2.9–26.0°
μ = 0.26 mm^{-1}
T = 294 (2) K
Block, colourless
0.32 × 0.30 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.920, T_{max} = 0.939
3112 measured reflections
2131 independent reflections
1578 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 8$
$l = -14 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.162$
S = 1.05
2131 reflections
165 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.104P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.85	2.658 (3)	171

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

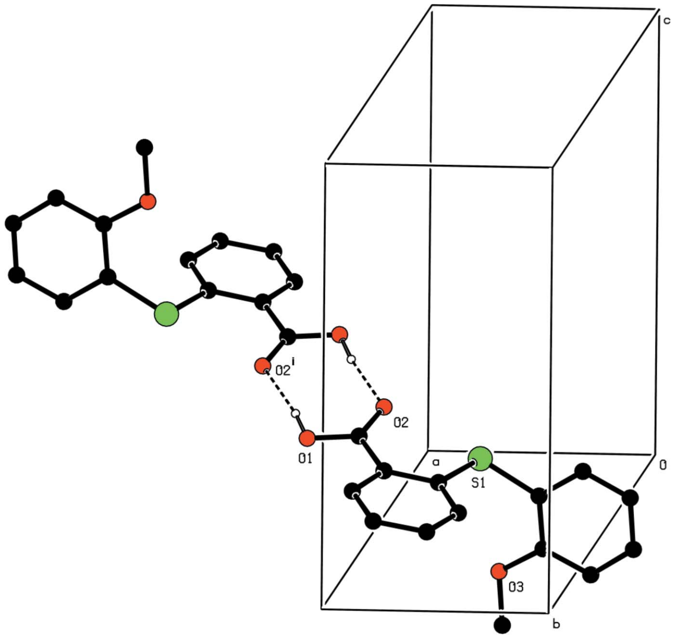

Figure 2
View showing the formation of the pseudo-dimer through O—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (i) $2 - x, 2 - y, 1 - z$.]

All H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H = 0.93 (aromatic) or 0.96 Å (methyl) and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C_{ar},O) and 1.5U_{eq}(methyl C).

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: *SHELXTL* (Bruker, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Mehta, N. B. & Brieaddy, L. E. (1997). US Patent No. 4056632.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wilson, A. A., Ginovart, N., Schmidt, M., Meyer, J. H., Threlkeld, P. G. & Houle, H. (2000). *J. Med. Chem.* **43**, 3103–3110.
Wilson, A. A. & Houle, S. (1999). *J. Labelled Compd. Radiopharm.* **42**, 1277–1288.
Younes, S., Labssita, Y., Baziard-Mouysset, G., Payard, M., Rettotri, M. C., Renard, P., Pfeiffer, B. & Caiqnard, D. H. (2000). *Eur. J. Med. Chem.* **35**, 107–121.