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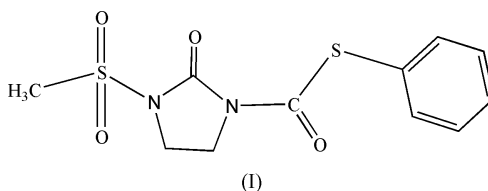
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Key indicatorsSingle-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.034
 wR factor = 0.092
Data-to-parameter ratio = 13.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**S-Phenyl 3-methanesulfonyl-2-oxoimidazol-
idine-1-carbothioate**

In the title compound, $\text{C}_{11}\text{H}_{12}\text{N}_2\text{O}_4\text{S}_2$, the five atoms of the imidazolidine ring are nearly coplanar, the average deviation being 0.0207 \AA . This ring makes a dihedral angle of $44.77(5)^\circ$ with the plane of the phenyl ring. The crystal structure is stabilized by three kinds of intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

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Thiol esters are important intermediates in organic synthesis and have been used, for example, as mild acyl transfer reagents (Mukaiyama *et al.*, 1973), as intermediates in the synthesis of ketones (McGarvey *et al.*, 1986) and in asymmetric aldol reactions (Kobayashi *et al.*, 1991). Thiol esters also constitute an important group of natural products (Halcomb *et al.*, 1995). Many show physiological activity and are widely applied in medicines and pesticides; examples include Timbensone, which is a corticoid antibiotic, and compounds such as 2-phenyl-1-ethyl (2*S*)-1-(3,3-dimethyl-1,2-dioxopentyl)-2-pyrrolidinedicarbothioate, used for the treatment of Parkinsonism (Hamiton & Li, 1999). The syntheses of the title compound, (I), and its derivatives have been reported (Su *et al.*, 2002). To extend this research, we report here the crystal structure of (I).



In (I), the r.m.s. deviation of the phenyl ring from planarity is 0.007 \AA , which indicates that atom S2 has little influence on phenyl ring planarity. The $\text{S}2-\text{C}5$ bond length is $1.777(18)\text{ \AA}$, similar to that found in triphenyltin thiobenzoate (Yin *et al.*,

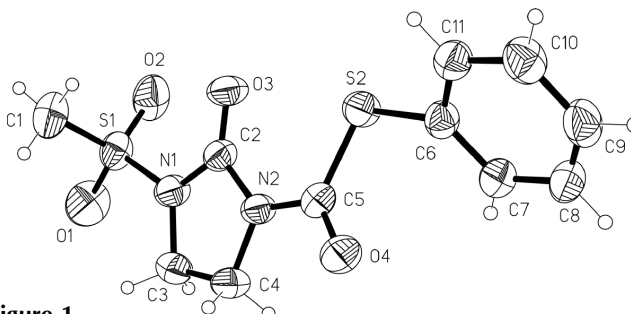


Figure 1
The molecular structure of (I), with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

2003), where the S—C bond length is 1.769 (9) Å. Moreover, the five atoms (N1, C2, N2, C3 and C4) of the imidazolidine ring are nearly coplanar, with an r.m.s. deviation of 0.021 Å. The dihedral angle between the imidazolidine and phenyl rings is 40.77 (5)°. In the crystal structure, there are three intermolecular C—H...O hydrogen bonds (Table 2), resulting in the formation of a three-dimensional network structure (Fig. 2).

Experimental

The title compound was synthesized by the reaction of 3-methanesulfonyl-2-oxoimidazolidine-1-carbonyl chloride (2.27 g, 0.01 mol) and benzenethiol (1.0 g, 0.01 mol) in the presence of toluene (20 ml) with active Zn powder as catalyst (0.65 g). The reaction was carried out under reflux for 6 h. Single crystals were obtained by recrystallization from tetrahydrofuran.

Crystal data

$C_{11}H_{12}N_2O_4S_2$	$D_x = 1.548 \text{ Mg m}^{-3}$
$M_r = 300.35$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3802 reflections
$a = 6.2189 (2) \text{ \AA}$	$\theta = 2.5\text{--}25.2^\circ$
$b = 16.0064 (6) \text{ \AA}$	$\mu = 0.42 \text{ mm}^{-1}$
$c = 12.9780 (4) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 93.967 (1)^\circ$	Block, colorless
$V = 1288.76 (8) \text{ \AA}^3$	$0.39 \times 0.36 \times 0.26 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART APEX area-detector diffractometer	2331 independent reflections
φ and ω scans	2080 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.017$
$T_{\text{min}} = 0.852$, $T_{\text{max}} = 0.898$	$\theta_{\text{max}} = 25.2^\circ$
6730 measured reflections	$h = -7 \rightarrow 7$
	$k = -19 \rightarrow 11$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.4005P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
2331 reflections	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
173 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

S1—O1	1.4166 (16)	O4—C5	1.207 (2)
S1—O2	1.4172 (16)	N1—C2	1.382 (2)
S1—N1	1.6618 (15)	N1—C3	1.463 (2)
S1—C1	1.750 (2)	N2—C5	1.386 (2)
S2—C6	1.7767 (18)	N2—C2	1.389 (2)
S2—C5	1.7777 (18)	N2—C4	1.466 (2)
O3—C2	1.199 (2)	C3—C4	1.522 (3)
O1—S1—O2	119.95 (11)	C5—N2—C4	119.46 (15)
O1—S1—N1	104.88 (9)	C2—N2—C4	112.86 (14)
O2—S1—N1	108.15 (8)	O3—C2—N1	126.83 (17)
O1—S1—C1	109.37 (11)	O3—C2—N2	127.05 (17)
O2—S1—C1	109.30 (12)	N1—C2—N2	106.10 (15)
N1—S1—C1	103.95 (9)	N1—C3—C4	103.49 (14)
C6—S2—C5	100.64 (8)	N2—C4—C3	103.78 (14)
C2—N1—C3	113.52 (15)	O4—C5—N2	119.79 (17)
C2—N1—S1	123.50 (13)	O4—C5—S2	124.83 (14)
C3—N1—S1	122.80 (12)	N2—C5—S2	115.33 (12)
C5—N2—C2	127.64 (15)		

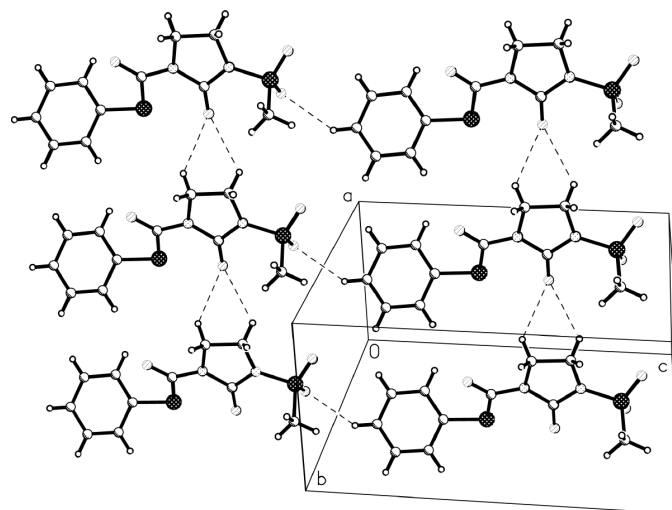


Figure 2

The three-dimensional network of (I). H bonds are indicated by dashed lines.

Table 2

Hydrogen-bonding geometry (Å, °).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
C3—H3A...O3 ⁱ	0.97	2.59	3.247 (2)	125
C4—H4B...O3 ⁱ	0.97	2.56	3.244 (2)	128
C9—H9...O2 ⁱⁱ	0.93	2.51	3.240 (2)	136

Symmetry codes: (i) $1 + x, y, z$; (ii) $x, y, z - 1$.

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with $Csp^2\text{—}H = 0.93 \text{ \AA}$ and $U_{\text{iso}} = 1.2U_{\text{eq}}$ (parent atom), and $Csp^3\text{—}H = 0.96$ or 0.97 \AA and $U_{\text{iso}} = 1.5U_{\text{eq}}$ (parent atom).

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: XP (Bruker, 2002); software used to prepare material for publication: SHELXL97.

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