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Dimethyl *N*-(4-phenyl-1,3-thiazol-2-yl)-dithioimidocarbonate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.106
Data-to-parameter ratio = 35.0

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

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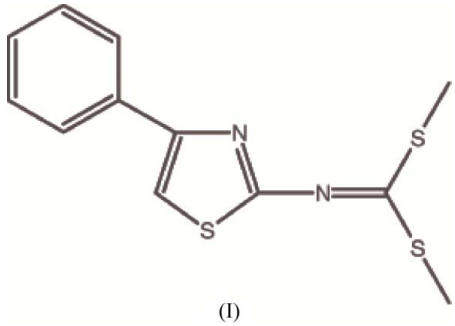
The title compound, $C_{12}H_{12}N_2S_3$, was synthesized by the reaction of CS_2 and CH_3I with 2-amino-4-phenyl-1,3-thiazole in the presence of concentrated aqueous NaOH. The bond lengths and angles are normal. The crystal packing is stabilized by van der Waals forces.

Comment

N-Substituted and *N*,*N*-disubstituted dithiocarbamate derivatives exhibit antibacterial, antiviral and antifungal activities (Kaplancikli *et al.*, 2004; Servi *et al.*,2005). The reaction of CS_2 and CH_3I with heteroaromatic amines in the presence of concentrated aqueous NaOH leads to the formation of methyl *N*-arylthiocarbamates and dimethyl *N*-aryldithiocarbonimidates, which allow the synthesis of 2-arylamino-2-imidazolines and 2-arylamino-1*H*-benzimidazoles (Genç & Servi, 2005; Servi, 2002; Garin *et al.*, 1990; Melendez *et al.*, 1991). We present here the crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), all bond lengths and angles are normal (Allen *et al.*, 1987) and correspond to those observed in the related

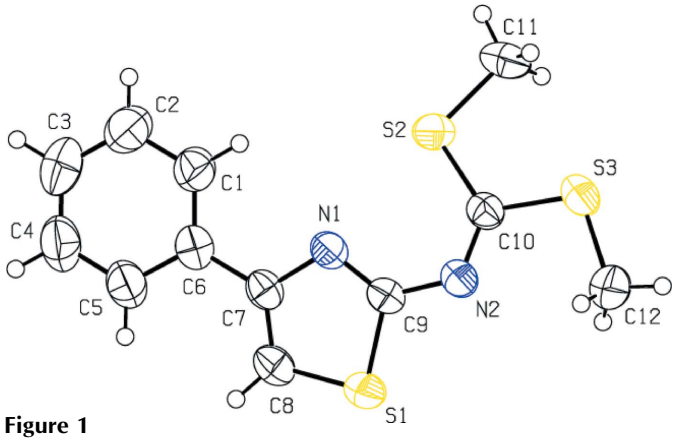


Figure 1
View of (I) showing the atomic labelling and displacement ellipsoids drawn at the 50% probability level.

compounds (Akkurt *et al.*, 2005; Öztürk Yıldırım *et al.*, 2006). In the absence of classical hydrogen bonds, the crystal packing (Fig. 2) is stabilized by van der Waals forces.

Experimental

To a well stirred cold solution of 2-amino-4-phenyl-1,3-thiazole (0.05 mol) in DMF (20 ml) was added aqueous NaOH (20 *M*, 4 ml), carbon disulfide (15 ml, 0.1 mol) and methyl iodide (0.1 mol) in sequence at intervals of 30 min, and stirring was continued for 2–4 h. The mixture was then poured into cold water and the resulting solid was washed with water and recrystallized from DMF/EtOH (3:7). The title compound was obtained in 82% yield (m.p. 367 K).

Crystal data

$C_{12}H_{12}N_2S_3$
M_r = 280.45
Orthorhombic, *Pbca*
a = 7.6626 (1) Å
b = 18.2969 (3) Å
c = 19.4176 (3) Å
V = 2722.38 (7) Å^3
Z = 8
D_x = 1.368 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 293 K
Block, colourless
0.60 × 0.32 × 0.27 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
39182 measured reflections
5387 independent reflections
3036 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 33.8°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.106
S = 1.01
5387 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.1433P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

H atoms were positioned geometrically, with C—H = 0.93–0.96 Å, and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

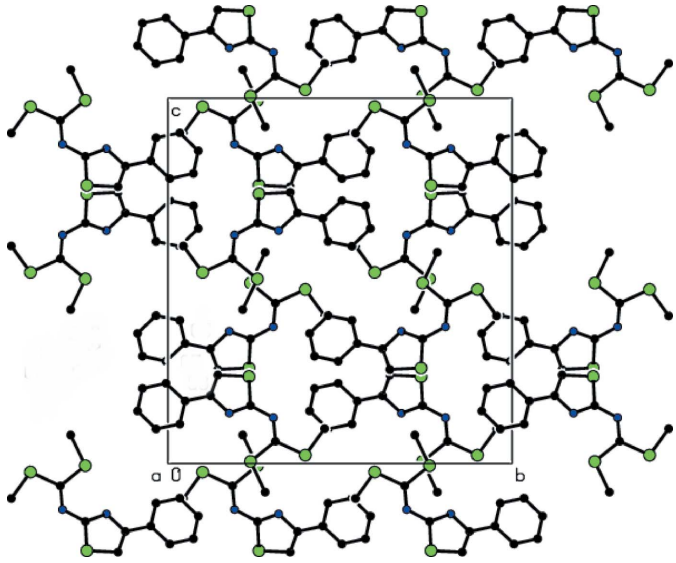


Figure 2
The crystal packing, viewed down the *a* axis. H atoms have been omitted.

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