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6-(Methylsulfanyl)-2-phenylthiazolo[5,4-*b*]pyridine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.052
wR factor = 0.201
Data-to-parameter ratio = 15.2

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

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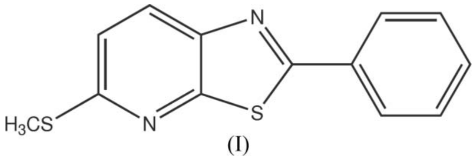
The molecule of the title compound, $C_{13}H_{10}N_2S_2$, is approximately planar, the thiazolopyridine ring system being slightly twisted from the phenyl ring. The molecules are stacked along the *b* axis through π–π interactions.

Comment

Thiazolopyridine derivatives have been widely studied because of their analgesic, antipyretic and anti-inflammatory properties (Couture & Grandclaudon, 1985, 1987). Most of them have a methyl or methoxy substituent attached to the pyridine ring of the thiazolopyridine unit (Kaigorodova, Osipova *et al.*, 2004; Kaigorodova, Vasilin *et al.*, 2004). As part of an investigation of the antitumor properties of the thiazolopyridine analogs, we report the synthesis and structure of the title compound, (I), containing a methylsulfanyl substituent attached to the pyridine ring.



(I)

The molecular structure is approximately planar (Fig. 1), the thiazolopyridine ring system and the phenyl ring being slightly twisted by 9.685 (12)°, which is comparable to the corresponding angles reported in 5-dimethylamino-2-phenyl-4,7-dioxobenzothiazole (Lyon *et al.*, 1999) and 5-benzyl-2-phenyl-4-tolylthiazole (Bart *et al.*, 1978). The bond distances of S1—C7 and S1—C12 in (I) (Table 1) are a little longer than those in other thiazolo derivatives (Kasim & Yamin, 2005; Cui *et al.*, 2005). The methylsulfanyl group is slightly twisted from the pyridine ring plane with a C13—S2—C11—N2 torsion angle of 6.0 (4)°. The S2—C11 bond is longer than the reported values of 1.713 (2)–1.765 (2) Å (Low *et al.*, 1996*a*,*b*; Yu *et al.*, 1996), while the S2—C13 bond is a little shorter than the corresponding values of 1.795 (2) Å (Lipinska, 2005) and 1.823 (2) Å (Low *et al.*, 1996*b*). In the crystal structure, the molecules are stacked along the *b* axis, forming a column in which the short intermolecular contact between the thiazole S1/C7/N1/C8/C12 and phenyl C1–C6 rings indicates the existence of a π–π stacking interaction [$Cg1\cdots Cg2^{i}$ = 3.759 (2) Å, where *Cg*1 and *Cg*2 are the centroids of the thiazole and phenyl rings, respectively; symmetry code: (i) *x*, −1 + *y*, *z*].

Experimental

To an anhydrous xylene solution (10 ml) of methyl methylthiomethyl sulfoxide (8 mmol, 0.1 g) was added sodium hydride (8 mmol, 0.032 g) under a nitrogen atmosphere. The mixture was heated to 337 K and 2-phenyl-6-chlorothiazolo[5,4-*b*]pyridine (0.2 g) was added. After refluxing the solution for 8 h, the reaction mixture was poured into water (50 ml). The product was extracted with ethyl acetate and the organic layer was dried with magnesium sulfate. The solvent was removed under reduced pressure and the residual product was chromatographed to give pure (I) (yield 70%, 0.14 g). Single crystals suitable for X-ray diffraction were obtained from an *n*-hexane solution at room temperature.

Crystal data

$C_{13}H_{10}N_2S_2$
$M_r = 258.35$
Monoclinic, $P2_1/c$
$a = 19.467$ (4) Å
$b = 5.063$ (1) Å
$c = 12.152$ (2) Å
$\beta = 90.09$ (3)°
$V = 1197.7$ (4) Å^3

$Z = 4$
$D_x = 1.433$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.42$ mm^{-1}
$T = 293$ (2) K
Plate, colorless
0.40 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.850$, $T_{\max} = 0.959$
2417 measured reflections

2346 independent reflections
1608 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 26.0°$
3 standard reflections every 200 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.202$
$S = 1.05$
2346 reflections
154 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.12P)^2 + 0.55P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.37$ e Å^{-3}
$\Delta\rho_{\min} = -0.41$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

S1—C12	1.740 (4)	S2—C11	1.763 (4)
S1—C7	1.750 (4)	S2—C13	1.789 (5)
C12—S1—C7	88.88 (19)	C11—S2—C13	102.4 (2)

All H atoms were located in a difference Fourier map, and then they were placed in idealized positions (C—H = 0.93–0.96 Å) and treated as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}$(methyl C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: *SHELXL97*.

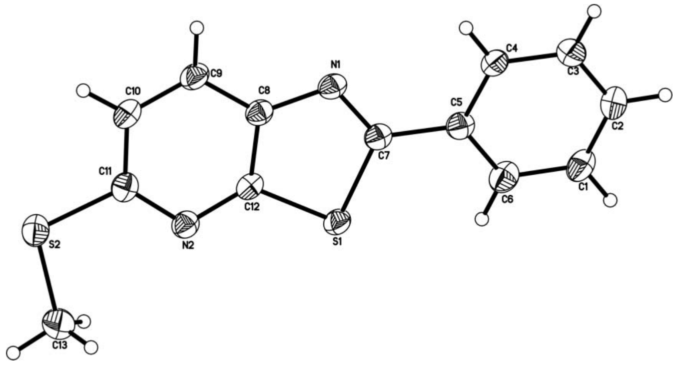


Figure 1
The molecular structure of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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