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5-Methyl-2-methylsulfanyl-7-phenylpyrazolo-[1,5-*a*]pyrimidine-3-carbonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.122
Data-to-parameter ratio = 15.7

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

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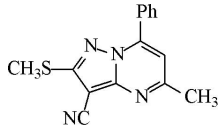
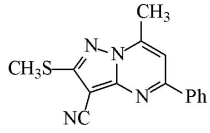
The pyrazolo[1,5-*a*]pyrimidine ring system of the title compound, $C_{15}H_{12}N_4S$, is essentially planar and the dihedral angle between the plane of the pyrazolo[1,5-*a*]pyrimidine system and the plane of the phenyl ring is 134.6 (7)°.

Comment

Pyrazolo[1,5-*a*]pyrimidines are of pharmacological importance as purine analogues and, used in the treatment of hyperuricaemia and gout, inhibit *de novo* purine biosynthesis and xanthine oxidase (El-Gaby *et al.*, 2000; Elnagdi *et al.*, 1987). In our recent research, a series of derivatives have been synthesized in order to look for new compounds having herbicidal activity (Sawhney *et al.*, 1981). Cyclization of 5-aminopyrazole with a dione compound gives the desired pyrazolo[1,5-*a*]pyrimidine, which results in the production of two positional isomers, (I) and (II).



(I)



(II)

The structure of (I), reported here (Fig. 1), allowed us to investigate the relationship between structure and herbicidal activity. There are three planes in (I); these are defined as *p*1 (C1/C2/C3/N1/N2), *p*2 (C3/C4/C5/C6/N2/N3) and *p*3 (C9/C10/C11/C12/C13/C14). The dihedral angles between the planes are 0.4 (3)° for *p*1/*p*2, 134.7 (2)° for *p*1/*p*3 and 134.6 (3)° for *p*2/*p*3.

Experimental

1-Phenylbutane-1,3-dione (0.32 g, 2 mmol) in ethanol (5 ml) was added to a solution of 5-amino-3-methylsulfanyl-1*H*-pyrazole-4-carbonitrile (0.31 g, 2 mmol) in ethanol (15 ml) containing a few drops of acetic acid. The mixture was refluxed for 5 h then cooled to room temperature, and the crude product (0.5 g, 89.3%) was obtained without further purification. The isomers were separated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3/1 (*v*/*v*) and the ratio of the isomers was 59.2:40.8 for (I):(II).

Crystal data

$C_{15}H_{12}N_4S$
M_r = 280.35
Monoclinic, $P2_1/c$
a = 8.819 (3) Å
b = 7.822 (3) Å
c = 20.465 (8) Å
β = 96.507 (7)°
V = 1402.6 (9) Å^3
Z = 4
D_x = 1.328 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 778 reflections
θ = 3.2–23.2°
μ = 0.23 mm^{-1}
T = 293 (2) K
Block, colourless
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2880 independent reflections
φ and ω scans	1655 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.047$
$T_{min} = 0.863$, $T_{max} = 1.000$	$\theta_{max} = 26.5^{\circ}$
7758 measured reflections	$h = -11 \rightarrow 9$
	$k = -9 \rightarrow 9$
	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.0043P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.051$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.122$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.24$ e Å^{-3}
2880 reflections	
183 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.735 (3)	N4—C7	1.139 (3)
N1—N2	1.376 (3)	C2—C7	1.409 (4)
N2—C4	1.367 (3)	C4—C5	1.363 (3)
N2—C3	1.381 (3)	C4—C9	1.467 (3)
C1—S1—C8	101.26 (13)	C5—C4—N2	114.7 (2)
N1—N2—C3	112.53 (19)	N4—C7—C2	179.1 (3)
C1—N1—N2—C3	−1.0 (2)	C5—C4—C9—C14	−43.9 (4)

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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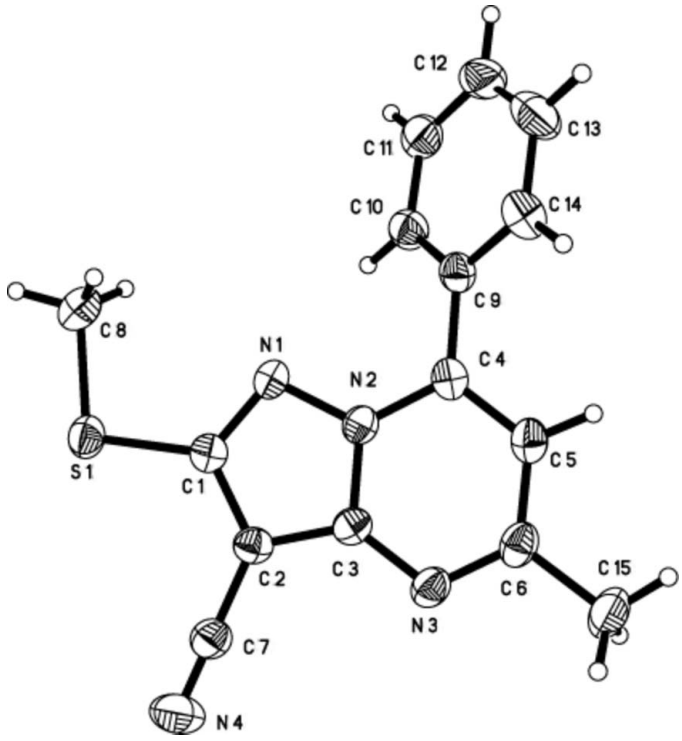

Figure 1
A view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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