graphics: *SHELXTL/PC* (Sheldrick, 1990*b*). Software used to prepare material for publication: *SHELXL*93. Geometric calculations: *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: AS1160). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2-(4-Hydroxyphenyl)benzothiazole

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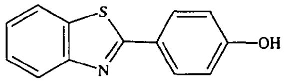
Abstract

The planar thiazole ring of the title compound, $C_{13}H_9NOS$, makes an angle of 1.39 (7)° with the benzene plane. The phenyl ring is not coplanar with the benzothiazole moiety; the dihedral angle between the thiazole and phenyl rings is 18.49 (6)°.

Comment

The thiazole ring of the title compound, (I), prepared in our laboratory, is planar and makes an angle of 1.39 (7)° with the benzene plane. The phenyl ring is twisted from the benzothiazole moiety about the C(1)—C(7) bond; the torsion angle C(6)—C(1)—C(7)—S is 19.4 (3)°.



(I)

A comparison between the title structure and those of known thiazole derivatives (Caranoni & Reboul, 1982; Prout & Miao, 1982; Bolognesi, Catellani, Destri & Porzio, 1987*a*,*b*) reveals no significant differences, either in bond lengths or in bond angles. A close intermolecular contact [2.759 (8) Å] exists between the N and O($1 - x$, $\frac{1}{2} + y$, $\frac{3}{2} - z$) atoms.

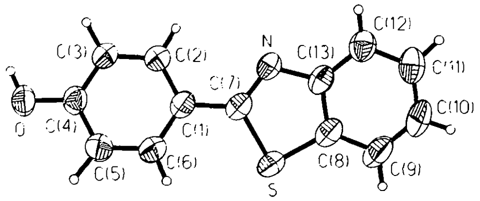


Fig. 1. View of the title compound with atomic numbering. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

Crystal data

$C_{13}H_9NOS$
$M_r = 227.3$
Orthorhombic
Pbca
$a = 13.188\ (2)$ Å
$b = 7.722\ (1)$ Å
$c = 21.178\ (3)$ Å
$V = 2156.7\ (6)$ Å^3
$Z = 8$
$D_x = 1.400$ Mg m^{-3}
$D_m = 1.391$ Mg m^{-3}
D_m measured by flotation

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 50 reflections
$\theta = 7.5$–17.5°
$\mu = 0.274$ mm^{-1}
$T = 298$ K
Plate
0.8 × 0.2 × 0.1 mm
Colourless

Data collection

Siemens *P*4 diffractometer
$2\theta/\theta$ scans
Absorption correction: refined from ΔF (Ugozzoli, 1987)
$T_{\min} = 0.797$, $T_{\max} = 0.986$
2373 measured reflections
2373 independent reflections
1781 observed reflections [$F > 4\sigma(F)$]

$\theta_{\max} = 27.5°$
$h = 0 \rightarrow 17$
$k = 0 \rightarrow 8$
$l = 0 \rightarrow 27$
2 standard reflections monitored every 100 reflections
intensity decay: not significant

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Refinement

Refinement on F
$R = 0.0371$
$wR = 0.0573$
$S = 1.34$
1781 reflections
181 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F) + 0.0010F^2]$
$(\Delta/\sigma)_{\max} = 0.009$
$\Delta\rho_{\max} = 0.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *SHELXTL/PC* (Sheldrick, 1990)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
S	0.7175 (1)	0.0365 (1)	0.5606 (1)	0.065 (1)
N	0.5365 (1)	0.1280 (2)	0.5925 (1)	0.047 (1)
O	0.6428 (1)	−0.2793 (2)	0.8496 (1)	0.068 (1)
C(1)	0.6231 (1)	−0.0346 (2)	0.6756 (1)	0.048 (1)
C(2)	0.5358 (1)	−0.0729 (3)	0.7097 (1)	0.050 (1)
C(3)	0.5404 (1)	−0.1513 (3)	0.7679 (1)	0.051 (1)
C(4)	0.6332 (1)	−0.1971 (3)	0.7936 (1)	0.052 (1)
C(5)	0.7212 (1)	−0.1577 (4)	0.7606 (1)	0.071 (1)
C(6)	0.7155 (1)	−0.0781 (3)	0.7025 (1)	0.068 (1)
C(7)	0.6161 (1)	0.0479 (2)	0.6136 (1)	0.048 (1)
C(8)	0.6469 (2)	0.1509 (3)	0.5058 (1)	0.055 (1)
C(9)	0.6736 (2)	0.2054 (3)	0.4455 (1)	0.072 (1)
C(10)	0.6032 (2)	0.2957 (3)	0.4113 (1)	0.070 (1)
C(11)	0.5073 (2)	0.3296 (3)	0.4352 (1)	0.066 (1)
C(12)	0.4805 (2)	0.2756 (3)	0.4949 (1)	0.058 (1)
C(13)	0.5510 (1)	0.1868 (2)	0.5307 (1)	0.048 (1)

Table 2. *Selected geometric parameters* (Å, °)

S—C(7)	1.747 (2)	S—C(8)	1.732 (2)
N—C(7)	1.297 (2)	N—C(13)	1.397 (2)
O—C(4)	1.350 (2)	C(1)—C(2)	1.391 (2)
C(1)—C(6)	1.386 (3)	C(1)—C(7)	1.464 (2)
C(2)—C(3)	1.375 (3)	C(3)—C(4)	1.385 (2)
C(4)—C(5)	1.389 (3)	C(5)—C(6)	1.377 (3)
C(8)—C(9)	1.389 (3)	C(8)—C(13)	1.399 (3)
C(9)—C(10)	1.369 (3)	C(10)—C(11)	1.387 (4)
C(11)—C(12)	1.379 (3)	C(12)—C(13)	1.382 (3)
C(7)—S—C(8)	89.6 (1)	C(7)—N—C(13)	111.5 (1)
C(2)—C(1)—C(6)	117.6 (2)	C(2)—C(1)—C(7)	120.4 (2)
C(6)—C(1)—C(7)	122.0 (2)	C(1)—C(2)—C(3)	121.5 (2)
C(2)—C(3)—C(4)	120.3 (2)	O—C(4)—C(3)	123.3 (2)
O—C(4)—C(5)	117.7 (2)	C(3)—C(4)—C(5)	119.0 (2)
C(4)—C(5)—C(6)	120.1 (2)	C(1)—C(6)—C(5)	121.6 (2)
S—C(7)—N	115.0 (1)	S—C(7)—C(1)	120.3 (1)
N—C(7)—C(1)	124.6 (2)	S—C(8)—C(9)	129.4 (2)
S—C(8)—C(13)	109.5 (1)	C(9)—C(8)—C(13)	121.1 (2)
C(8)—C(9)—C(10)	118.0 (2)	C(9)—C(10)—C(11)	121.4 (2)
C(10)—C(11)—C(12)	120.8 (2)	C(11)—C(12)—C(13)	118.8 (2)
N—C(13)—C(8)	114.4 (2)	N—C(13)—C(12)	125.7 (2)
C(8)—C(13)—C(12)	119.9 (2)		

The structure was solved by direct methods and refined by the full-matrix least-squares method. All H atoms were located from the difference Fourier map. The *SHELXTL/PC* (Sheldrick, 1990) program package was used for all calculations.

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: LI1128). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(*Z*)-Ethyl 2-Cyano-3-methylsulfinyl-3-methylthiopropenoate

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Abstract

The title compound, $C_8H_{11}NO_3S_2$, is shown to be formed in the oxidation of ethyl 2-cyano-3,3-bis(methylthio)propenoate with 3-chloroperoxybenzoic acid. The compound contains an $(S_2)C{=}C(C_2)$ unit which is not exactly planar, as indicated by atomic deviations of ±0.130 (1) Å from the least-squares plane through these six atoms. The C—S bond lengths are unexceptional but the bond between the $CH_3(O)S$— group and the alkene C atom is slightly longer than expected [1.837 (3) Å].

Comment

Ketene dithioacetal derivatives (Söderbäck, 1963) are well known reagents for the preparation of different types of heterocyclic compounds. For example, the synthesis of different lactones, pyrazoles and isoxazole derivatives has been reported (Tominaga, Ushirogochi, Matsuda & Kobayashi, 1984; Ram, Haque, Singh, Hussaini & Shoeb, 1993; Ram, Hussaini, Singh &