programs used in this work are listed in reference 11 of Gadol & Davis (1982).

Related literature. Appropriately substituted 1,2,3-cyclopropanes have potential uses as replacements for the dipeptide unit in the design of new enzyme inhibitors and peptide hormone antagonists. A general method for the stereoselective synthesis of 1,2,3-trisubstituted cyclopropanes has been reported (Martin, Austin & Oalmann, 1990).

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Structure of 1-(2-Methyl-2,3-dihydrobenzothiazol-2-yl)-2-propanone

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Abstract. $C_{11}H_{13}NOS$, $M_r = 207{\cdot}29$, monoclinic, $P2_1/c$, $a = 8{\cdot}433\,(2)$, $b = 12{\cdot}932\,(1)$, $c = 10{\cdot}503\,(3)$ Å, $\beta = 111{\cdot}77\,(1)^\circ$, $V = 1063{\cdot}7\,(7)$ Å^3, $Z = 4$, $D_m = 1{\cdot}307$ (flotation in nitromethane/chloroform), $D_x = 1{\cdot}294$ Mg m^{-3}, $\lambda(\text{Mo }K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}26$ mm^{-1}, $F(000) = 440$, $T = 298$ K, $R = 0{\cdot}0574$ for 1752 observed reflections $[I > 2{\cdot}5\sigma(I)]$. The phenyl ring is coplanar with the S and N atoms of the fused five-membered ring with torsion angles S—C(6)—C(1)—C(2) of −178·0 (2) and N—C(1)—C(6)—C(5) of 176·1 (3)°, but C(7) is displaced from the mean plane of the phenyl ring by 0·322 (2) Å. The S—C(6) distance [1·748 (2) Å] is less than that of S—C(7) [1·846 (2) Å] owing to the fact that C(7) is sp^3 hybridized whereas C(6) is part of the aromatic ring. Similar arguments pertain to the difference in the N—C distances; N—C(1) = 1·388 (3) and N—C(7) = 1·463 (3) Å.

Experimental. The title compound was prepared by a previously reported method (Cefalu, Bosco, Bonati, Maggio & Barbieri, 1970). Preliminary data obtained from Weissenberg and Buerger precession photographs yielded approximate cell dimensions and showed monoclinic symmetry, space group $P2_1/c$. Data collection on a crystal 0·3 × 0·2 × 0·2 mm was performed on a Syntex $P2_1$ diffractometer in $2\theta/\theta$ mode ($0 < h < 10$, $0 < k < 14$, $-12 < l < 12$) out to 2θ(max.) of 52·2°. Variable scan speed of 5·0–29·3° min^{-1} was used. Lattice parameters refined using 30 reflections in the range $35 < 2\theta < 45^\circ$. Standard reflection $0\bar{1}1$ checked every 50 reflections: no significant deviation. Data were corrected for Lorentz and polarization effects. 2317 reflections were collected, 2070 unique ($R_{\text{int}} = 0{\cdot}0807$), of which 1752 observed reflections with $I > 2{\cdot}5\sigma(I)$ were used for refinement of the structure. Structure solved by direct methods, *SHELXS86* (Sheldrick, 1986) and refined using *SHELX76* (Sheldrick, 1976). Scattering factors for C, H, N, O and S inlaid in *SHELX76*.

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Table 1. *Atomic coordinates* (× 10^4) *and* B_{eq} (Å^2) *values with e.s.d.'s in parentheses*

$B_{eq} = 8\pi^2(U_{11} + U_{22} + U_{33})/3$.

	x	y	z	B_{eq}
S	2553 (1)	8630 (1)	287 (1)	3·48 (3)
N	3142 (3)	8409 (2)	−1965 (2)	3·57 (9)
C(1)	1425 (3)	8662 (2)	−2373 (2)	3·29 (9)
C(2)	302 (4)	8811 (2)	−3696 (3)	4·26 (11)
C(3)	−1351 (4)	9139 (2)	−3920 (3)	4·57 (12)
C(4)	−1871 (4)	9301 (2)	−2853 (3)	4·58 (13)
C(5)	−759 (3)	9144 (2)	−1516 (3)	3·89 (11)
C(6)	885 (3)	8827 (2)	−1289 (3)	3·17 (9)
C(7)	3860 (3)	8003 (2)	−567 (2)	3·08 (9)
C(8)	3682 (4)	6836 (2)	−540 (3)	3·91 (11)
C(9)	5710 (3)	8357 (2)	85 (2)	3·28 (10)
C(10)	6546 (3)	8221 (2)	1600 (2)	3·39 (10)
O	5770 (3)	7906 (2)	2281 (2)	4·93 (10)
C(11)	8387 (4)	8520 (2)	2235 (3)	4·49 (13)

Structure determination and refinement performed on IBM 4361/4381. Refinement by full-matrix least squares based on F with idealized riding H atoms (C—H 0·96 Å); anisotropic refinement of non-H atoms, isotropic refinement for H atoms. In order to correct the observed structure factors for absorption effects, the program *ABSORB* (Ugozzoli, 1987) was used (correction factors min.–max. 0·8443–0·9986). The final agreement factors were $R = 0·0547$, $wR = 0·0640$. Weight for every observed structure factor calculated according to $w = 6·5675/[\sigma^2(F) + 0·000311F^2]$ for which $S = 1·46$, $(\Delta/\sigma)_{max} = 0·008$, $\Delta\rho_{max} = 0·232$ and $\Delta\rho_{min} = -0·202$ e Å^{-3}. Geometrical calculations performed with *XANADU* (Roberts & Sheldrick, 1979) and illustrations drawn with *ORTEP* (Johnson, 1965). The atomic parameters for non-H atoms are given in Table 1.* Table 2 contains bond distances and angles, while the atom-labelling scheme is shown in Fig. 1.

Related literature. Charles & Frieser (1953) have demonstrated that the Schiff base, *N*-(2-mercaptophenyl)salicylideneamine, generated by condensing 2-aminothiophenol with salicylaldehyde is not the stable form of the uncoordinated molecule. At room temperature this Schiff base thermally converts to 2-(2-hydroxyphenyl)-2,3-dihydrobenzothiazole.
Cefalu *et al.* (1970) carried out the direct condensation of 2-aminothiophenol with acetylacetone resulting in a product which was only characterized spectroscopically. The X-ray structure of the product is reported herein.

Table 2. *Bond distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(6)—S	1·748 (2)	C(5)—C(4)	1·384 (4)
C(7)—S	1·846 (2)	C(6)—C(5)	1·379 (3)
C(1)—N	1·388 (3)	C(8)—C(7)	1·519 (4)
C(7)—N	1·463 (3)	C(9)—C(7)	1·523 (3)
C(2)—C(1)	1·375 (3)	C(10)—C(9)	1·493 (3)
C(6)—C(1)	1·390 (4)	O—C(10)	1·206 (3)
C(3)—C(2)	1·391 (4)	C(11)—C(10)	1·495 (4)
C(4)—C(3)	1·363 (5)		
C(7)—S—C(6)	91·1 (1)	C(5)—C(6)—C1	121·2 (2)
C(7)—N—C(1)	113·0 (2)	N—C(7)—S	103·3 (2)
C(2)—C(1)—N	126·4 (2)	C(8)—C(7)—S	110·3 (2)
C(6)—C(1)—N	113·9 (2)	C(8)—C(7)—N	111·6 (2)
C(6)—C(1)—C(2)	119·6 (2)	C(9)—C(7)—S	110·3 (2)
C(3)—C(2)—C(1)	119·0 (3)	C(9)—C(7)—N	108·5 (2)
C(4)—C(3)—C(2)	121·0 (3)	C(9)—C(7)—C(8)	112·4 (2)
C(5)—C(4)—C(3)	120·5 (3)	C(10)—C(9)—C(7)	116·4 (2)
C(6)—C(5)—C(4)	118·6 (3)	O—C(10)—C(9)	121·8 (2)
C(1)—C(6)—S	111·1 (2)	C(11)—C(10)—C(9)	116·6 (2)
C(5)—C(6)—S	127·7 (2)	C(11)—C(10)—O	121·7 (2)

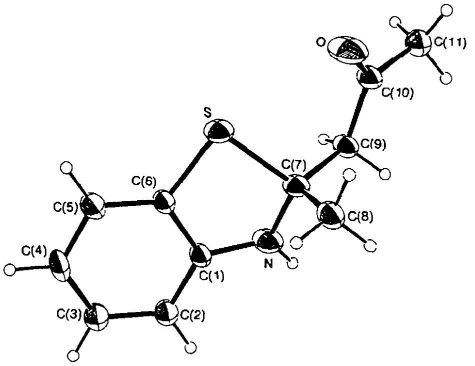

Fig. 1. A perspective view of the molecule.

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* Lists of structure factors, anisotropic thermal parameters, distances and angles involving H atoms, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53817 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.