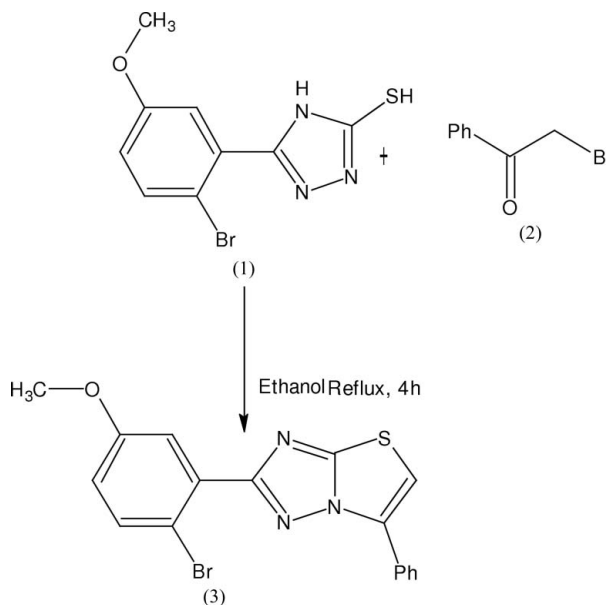


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Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.037
 wR factor = 0.087
Data-to-parameter ratio = 13.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.2-(2-Bromo-5-methoxyphenyl)-6-phenyl-1,3-thiazolo[3,2-*b*][1,2,4]triazoleThe molecule of the title compound, $\text{C}_{17}\text{H}_{12}\text{BrN}_3\text{OS}$, is essentially planar. Geometric parameters are in the normal ranges. There are two intramolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds.Received 29 August 2006
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Comment

The reaction of α -haloketones with 2-substituted 5-mercapto-1,2,4-triazoles may result in the formation of either the 2,5-disubstituted-thiazolo[3,2-*b*]-*s*-triazole or the 3,5-disubstituted thiazolo[3,2-*b*]-1,2,4-triazole or both (Berk *et al.*, 2001; Potts & Husain, 1971). The synthesis of thiazolo[3,2-*b*]-1,2,4-triazoles and the isomeric thiazolo[2,3-*c*]-1,2,4-triazoles, and their diuretic, antibacterial and antifungal activities, have been studied by Jag Mohan & Kiran (1988). In the present study, 5-(2-bromo-5-methoxyphenyl)-4*H*-1,2,4-triazole-3-thiol, (1), was refluxed with phenacyl bromide, (2), in ethanol to obtain 2-(2-bromo-5-methoxyphenyl)-6-aryl-1,3-thiazolo[3,2-*b*]-[1,2,4]triazole, (3) (see scheme). We present here the crystal structure of (3).

A perspective view of compound (3) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November 2005, updated August 2006; MOGUL, Version 1.1; Allen, 2002). The molecule is essentially planar (r.m.s. deviation for all non-H atoms is 0.059 Å).

The molecular conformation of (3) is stabilized by two intramolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds (Table 1).

Experimental

For the synthesis of compound (3), 5-(2-bromo-5-methoxyphenyl)-4*H*-1,2,4-triazole-3-thiol (2.86 g, 0.01 mol) and the appropriate 2-bromo-1-phenylethanone (2 g, 0.01 mol) were refluxed in ethanol for 4 h. The progress of the reaction was monitored by thin-layer chromatography. After completion of the reaction, the reaction mixture was cooled and the precipitated solid was filtered off. The solid obtained was recrystallized from a methanol–acetone solvent mixture (1:1). The compound was obtained as creamish crystals in 48% yield (m.p. 483 K). Analysis for C₁₇H₁₂BrN₃OS, found (calculated): C 52.80 (52.86), H 3.07 (3.13), N 10.72 (10.88)%. Spectroscopic data: IR (KBr, ν , cm⁻¹): 3118 and 3070 (–CH), 1475 (–C=N–), 734 (C–Br).

Crystal data

C ₁₇ H ₁₂ BrN ₃ OS	$Z = 8$
$M_r = 386.27$	$D_x = 1.669 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 14.9271 (13) \text{ \AA}$	$\mu = 2.82 \text{ mm}^{-1}$
$b = 10.9247 (13) \text{ \AA}$	$T = 173 (2) \text{ K}$
$c = 18.8582 (16) \text{ \AA}$	Plate, colourless
$V = 3075.3 (5) \text{ \AA}^3$	$0.32 \times 0.16 \times 0.08 \text{ mm}$

Data collection

Stoe IPDS II two-circle diffractometer	10330 measured reflections
ω scans	2883 independent reflections
Absorption correction: multi-scan (<i>MULABS</i> ; Spek, 2003; Blessing, 1995)	2189 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.466$, $T_{\max} = 0.806$	$R_{\text{int}} = 0.064$
	$\theta_{\text{max}} = 25.6^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.087$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.98$	$\Delta\rho_{\text{max}} = 0.55 \text{ e \AA}^{-3}$
2883 reflections	$\Delta\rho_{\text{min}} = -0.80 \text{ e \AA}^{-3}$
210 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	(Sheldrick, 1997)
	Extinction coefficient: 0.0046 (4)

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C26–H26 \cdots N8	0.95	2.40	2.788 (4)	104
C12–H12 \cdots N6	0.95	2.35	3.040 (4)	129

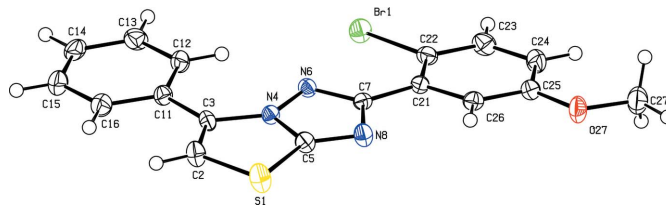


Figure 1

The molecular structure of compound (3), with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

H atoms were found in a difference map but they were subsequently refined using a riding model, with C–H = 0.95 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or C–H = 0.98 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$. The methyl group was allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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