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2-(2-Bromo-5-methoxyphenyl)-6-phenyl-1,3-thiazolo[3,2-*b*][1,2,4]triazole

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Key indicators

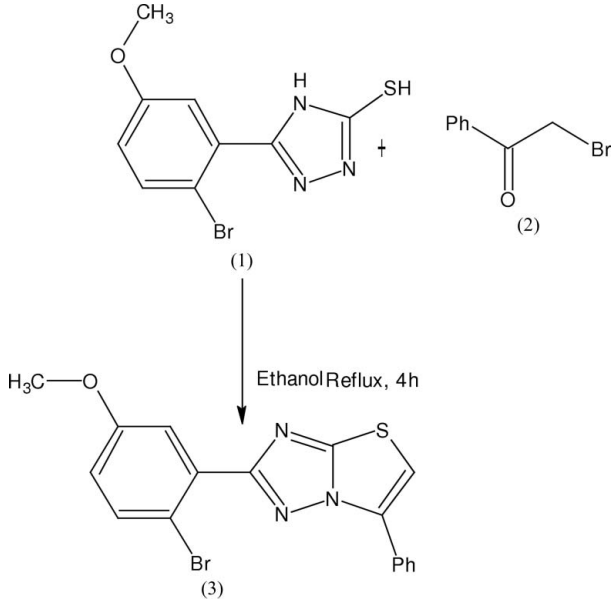
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.087
Data-to-parameter ratio = 13.7

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

The molecule of the title compound, $C_{17}H_{12}BrN_3OS$, is essentially planar. Geometric parameters are in the normal ranges. There are two intramolecular C—H···N hydrogen bonds.

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 C—H···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 $C_{17}H_{12}BrN_3OS$, 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

$C_{17}H_{12}BrN_3OS$
M_r = 386.27
Orthorhombic, *Pbca*
a = 14.9271 (13) Å
b = 10.9247 (13) Å
c = 18.8582 (16) Å
V = 3075.3 (5) Å^3
Z = 8
D_x = 1.669 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.82 mm^{-1}
T = 173 (2) K
Plate, colourless
0.32 × 0.16 × 0.08 mm

Data collection

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

Refinement

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

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C26—H26···N8	0.95	2.40	2.788 (4)	104
C12—H12···N6	0.95	2.35	3.040 (4)	129

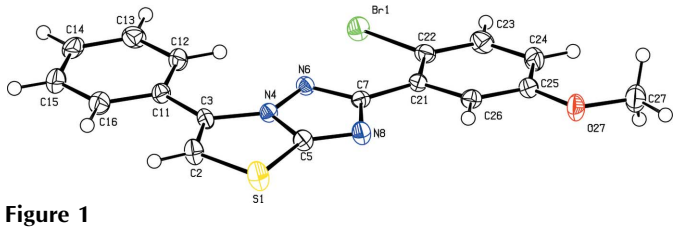


Figure 1
The molecular structure of compound (3), with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

H atoms were found in a difference map but they were subsequently refined using a riding model, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) or C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C_{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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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Berk, B., Aktay, Yesilada, G. E. & Ertan, M. (2001). *Pharmazie*, **56**, 613–616.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Jag Mohan & Kiran (1988). *Chim. Acta Turc.*, **16**, 91–98.
Potts, K. T. & Husain, S. (1971). *J. Org. Chem.* **36**, 10–13.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.