

3-(2-Bromo-5-methoxyphenyl)-5-methyl-1-(4-phenyl-1,3-thiazol-2-yl)-1H-1,2,4-triazole

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Key indicators

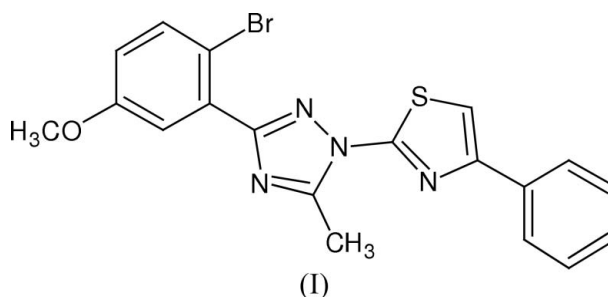
Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.034
 wR factor = 0.089
Data-to-parameter ratio = 14.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Molecules of the title compound, $\text{C}_{19}\text{H}_{15}\text{BrN}_4\text{OS}$, are essentially planar. Geometric parameters are in the usual ranges.

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Comment

Various 1,2,4-triazoles have been reported to possess antibacterial, antifungal, antitubercular, diuretic, antihypertensive and anti-inflammatory properties (Burch & Smith, 1966; Mir *et al.*, 1970; Goswami *et al.*, 1984; Demirayak *et al.*, 2000). On the basis of such findings, the 1,2,4-triazole nucleus has been incorporated into a wide variety of therapeutically interesting compounds to transform them into better drugs (Hendel & Raid, 1980). In view of the importance of substituted 1,2,4-triazoles, we attempted to synthesize 3-(2-bromo-5-methoxyphenyl)-5-phenyl[1,3]thiazolo[2,3-*c*][1,2,4]triazole. Instead, however, the title new triazole, (I), was formed by the reaction of 2-bromo-5-methoxy-*N'*-[4-(phenyl)-1,3-thiazol-2yl]benzohydrazide with acetonitrile. The crystal structure of (I) is reported here.



The molecular structure of compound (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Allen *et al.*, 1987). Molecules of (I) are essentially planar (r.m.s. deviation for all non-H atoms = 0.065 Å). The S atom of the thiazole ring is *trans* to the methyl group attached to the triazole ring.

Experimental

2-Bromo-5-methoxy-*N'*-[4-(phenyl)-1,3-thiazol-2yl]benzohydrazide (4.04 g, 0.01 mol) in POCl_3 (5 ml) and acetonitrile (15 ml) was refluxed for 10 h. The reaction mixture was then cooled, quenched in ice and the precipitated solid was filtered off. The solid obtained was recrystallized from a methanol–acetone mixture (1:1 *v/v*) (yield 58%; m.p. 435–437 K). Analysis for $\text{C}_{19}\text{H}_{15}\text{BrN}_4\text{OS}$: found (calculated): C 53.31 (53.40%), H 3.45 (3.54%), N 13.02 (13.11%).

Crystal data

C₁₉H₁₅BrN₄OS
M_r = 427.32
 Monoclinic, *P*2₁/*n*
a = 11.9585 (7) Å
b = 5.0552 (3) Å
c = 29.0105 (15) Å
 β = 90.863 (5)°
V = 1753.56 (17) Å³

Z = 4
D_x = 1.619 Mg m⁻³
 Mo *K*α radiation
 μ = 2.48 mm⁻¹
T = 173 (2) K
 Needle, colourless
 0.24 × 0.09 × 0.09 mm

Data collection

Stoe IPDS II two-circle diffractometer
 ω scans
 Absorption correction: multi-scan [MULABS (Spek, 2003; Blessing, 1995)]
T_{min} = 0.588, *T_{max}* = 0.808

18751 measured reflections
 3329 independent reflections
 2823 reflections with *I* > 2σ(*I*)
R_{int} = 0.085
 θ_{\max} = 25.7°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.034
wR(*F*²) = 0.089
S = 1.02
 3329 reflections
 237 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0561P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 $\Delta\rho_{\max} = 0.27 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.68 \text{ e \AA}^{-3}$

H atoms were found in a difference map but they were refined using a riding model, with C–H = 0.95 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C), or C–H = 0.98 Å and *U*_{iso}(H) = 1.5*U*_{eq}(C) for methyl H. The methyl groups were 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, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

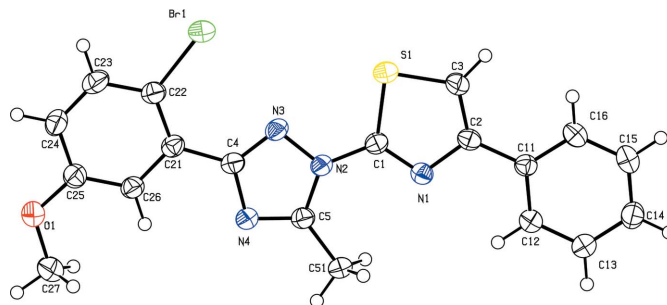


Figure 1
 The molecular structure of the title compound, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

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