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

H. S. Yathirajan,[a] K. K. Vijaya Raj,[b] B. Narayana,[b] B. K. Sarojini[c] and Michael Bolte[d]*

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [b]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, India, [c]Department of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and [d]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany

Correspondence e-mail: bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.089
Data-to-parameter ratio = 14.0

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

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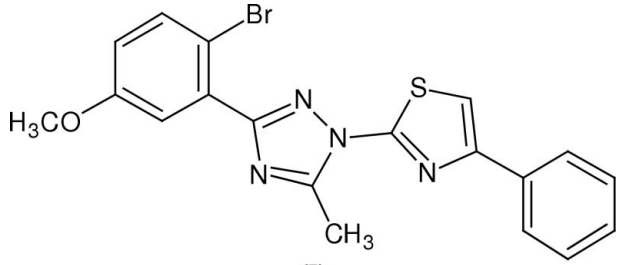
Molecules of the title compound, $C_{19}H_{15}BrN_4OS$, are essentially planar. Geometric parameters are in the usual ranges.

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.



(I)

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 $C_{19}H_{15}BrN_4OS$: found (calculated): C 53.31 (53.40%), H 3.45 (3.54%), N 13.02 (13.11%).

Crystal data

$C_{19}H_{15}BrN_4OS$
M_r = 427.32
Monoclinic, $P2_1/n$
a = 11.9585 (7) Å
b = 5.0552 (3) Å
c = 29.0105 (15) Å
β = 90.863 (5)°
V = 1753.56 (17) Å^3
Z = 4
D_x = 1.619 Mg m^{-3}
Mo $K\alpha$ 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 $I > 2\sigma(I)$
R_{int} = 0.085
θ_{max} = 25.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-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) = 1.2U_{eq}(C), or C—H = 0.98 Å and U_{iso}(H) = 1.5U_{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*.

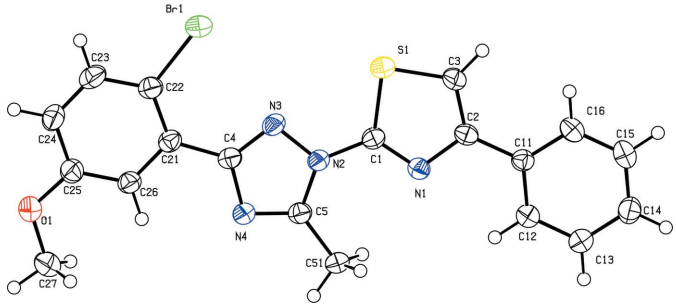


Figure 1
The molecular structure of the title compound, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

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