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N-(4-Methyl-3-phenyl-2,3-dihydro-1,3-thiazol-2-ylidene)benzamide

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.114
Data-to-parameter ratio = 15.0

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

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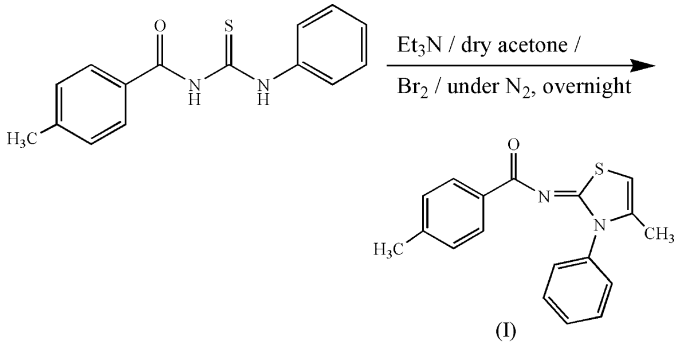
Geometric parameters of the title compound, $C_{18}H_{16}N_2OS$, are in the normal ranges. The phenyl ring is twisted by 68.22 (7)° out of the plane of the heterocycle.

Comment

2-Imino-1,3-thiazoline derivatives are associated with various pharmacological activities, for instance antimicrobial (Vittoria *et al.*, 1992), anti-inflammatory (Omar & Eshba, 1984), anti-histaminic (Chaudhary *et al.*, 1976), antihypertensive (Ragab *et al.*, 1993), hypnotic (Hassan *et al.*, 1998) and anticonvulsant activities (Turan-Zitouni *et al.*, 2002). Thiazolidinone derivatives of rhodanine are reported to have antibacterial, antiviral (Lee & Sim, 2000), pesticidal (Inamori *et al.*, 1998), anti-inflammatory (Habib *et al.*, 1997) and antidiabetic properties (Sing *et al.*, 2001). Thiazolines have been found to exhibit acaricidal, insecticidal and plant-growth regulatory activities (Hoelzel *et al.*, 1988) and have also been used for the identification of human cells with positive myeloperoxidase reactivity (Bonde & Gaikwad, 2004). 2-Phenylimino-1,3-thiazoline-4-acetanilides have shown significant antifungal activity against rice blast *Pyricularia oryzae*, and thus can be used as agrochemical fungicides (Bae *et al.*, 2005). We have already reported the synthesis of 2-aroylimino-3-aryl-4-methyl-1,3-thiazolines by base-catalysed cyclization of 1-aroyl-3-arylthioureas with acetone in the presence of bromine, which represent a new class of iminothiazolines (Saeed & Parvez, 2006).



(I)

A perspective view of the title compound is shown in Fig. 1. Geometric parameters are in the normal ranges (Allen *et al.*, 1987). The phenyl ring is twisted by 68.22 (7)° out of the plane of the heterocycle.

Experimental

2-(4-Methylbenzoylimino)-3-phenyl-4-methyl-1,3-thiazoline, (I), was prepared as follows. To a stirred solution of 1-(4-methylbenzoyl)-3-

phenylthiourea (0.002 mol) in acetone (20 ml) containing triethylamine (0.3 ml, 0.002 mol) was added dropwise a solution of bromine (0.002 mol) in acetone (10 ml) under nitrogen. After the addition was complete, the solution was stirred at room temperature overnight. The reaction mixture was filtered and concentrated to leave a crude solid. Recrystallization from aqueous ethanol afforded (I) as colourless crystals (yield 78%; m.p. 455 K). R_f 0.14 (hexane–EtOAc 7:3 *v*/*v*); IR (KBr, ν, cm^{-1}): 2938, 1673 (CO), 1600 (C═C), 1514, 1572 (C═N), 1265, 1152, 1050, 783, 736, 700; ^{1}H NMR ($CDCl_3$, δ, p.p.m.): 2.07 (*s*, 3H, C5-Me), 2.48 (*s*, 3H, Ar-Me), 6.45 (*s*, 1H, C4-H), 7.14 (2H, *AABB*), 7.24 (2H, *AABB*), 7.35 (2H, *AABB*), 7.67 (2H, *AABB*).

Crystal data

$C_{18}H_{16}N_2OS$
M_r = 308.39
Hexagonal, $R\overline{3}$
a = 18.8437 (14) Å
c = 23.561 (2) Å
V = 7245.3 (10) Å^3
Z = 18
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 173 (2) K
0.26 × 0.24 × 0.20 mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.939, T_{max} = 0.950
11573 measured reflections
3025 independent reflections
2336 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.114
S = 1.01
3025 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

H atoms were located in a difference synthesis but refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl})] using a riding model, with $C_{aromatic}$—H = 0.95 Å and C_{methyl}—H = 0.98 Å.

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*.

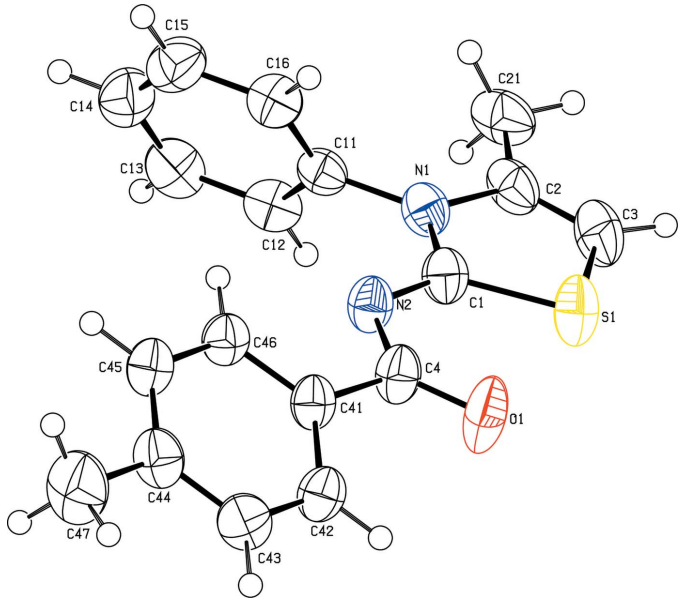


Figure 1
The molecular structure of compound (I), with displacement ellipsoids drawn at the 50% probability level.

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