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4-[(2-Methoxybenzylidene)amino]-1,5-dimethyl-2-phenyl-1*H*-pyrazolidin-3(2*H*)-one

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In the title compound, $C_{19}H_{19}N_3O_2$, the 2-methoxyphenyl ring is almost coplanar with the pyrazoline ring [dihedral angle 8.7 (4)°], while the phenyl ring forms a dihedral angle of 54.9 (2)° with the pyrazoline ring.

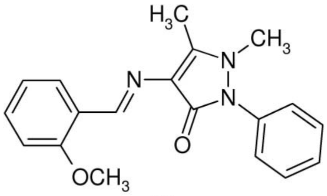
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.039
wR factor = 0.096
Data-to-parameter ratio = 8.0

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

Comment

The roles of antipyrine and antipyridine derivatives in biological processes have become a topic of study in recent years (Carlton *et al.*, 1995; Coolen *et al.*, 1999; Jiang *et al.*, 2000). The title compound, (I), is a new antipyrine Schiff base compound.



(I)

All bond lengths and angles in (I) are in agreement with those in similar antipyrine Schiff bases. The pyrazoline ring is essentially planar, the maximum deviation from the N1/N2/C1/C2/C3 mean plane being 0.042 (2) Å for N2. Atom O1 deviates from the N1/N2/C1/C2/C3 plane by 0.101 (5) Å, while atoms C4 and C5 deviate from it on the opposite side by 0.615 (6) Å and 0.122 (6) Å, respectively. The dihedral angle between the N1/N2/C1/C2/C3 plane and the C14–C19 phenyl ring is 54.9 (2)°. The N2—N1—C14—C19 and C1—N1—C14—C15 torsion angles are 149.6 (3) and 109.1 (4)°, respectively. The C6═N3 bond length of 1.280 (4) Å conforms to the expected value for a double bond (Allen *et al.*, 1987). Because of conjugation through this imine double bond, the pyrazoline ring and the substituted 2-methoxyphenyl ring (atoms C7–C12) are approximately coplanar [the mean deviation from the overall plane is 0.026 (3) Å]; the dihedral angle between the two rings is 8.7 (4)°. As expected, the molecule adopts a *trans* configuration about the C6═N3 bond.

Experimental

2-Methoxybenzaldehyde (0.1 mmol, 13.6 mg) and 4-aminoantipyrine (0.1 mmol, 20.3 mg) were dissolved in methanol (10 ml). The mixture was stirred for 30 min at room temperature to give a clear yellow solution. After allowing this solution to stand in air for 7 d, yellow block-shaped crystals of (I) were formed by slow evaporation of the solvent. The crystals were isolated by filtration, washed with methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$

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(yield 54%). Elemental analysis found: C 58.1, H 5.5%; calculated: C 58.2, H 5.6%.

Crystal data

$C_{19}H_{19}N_3O_2$
$M_r = 321.37$
Orthorhombic, $P2_12_12_1$
$a = 6.841$ (3) Å
$b = 14.021$ (6) Å
$c = 17.886$ (8) Å
$V = 1715.6$ (13) Å^3

$Z = 4$
$D_x = 1.244$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 298$ (2) K
Block, yellow
0.48 × 0.32 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.961$, $T_{\max} = 0.990$

8948 measured reflections
1761 independent reflections
1081 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.051$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.096$
$S = 1.01$
1761 reflections
220 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.4536P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ e Å^{-3}

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 (aromatic) or 0.96 Å (CH_3), and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(methyl C). The methyl groups were allowed to rotate about their local threefold axes. In the absence of significant anomalous scattering, 1262 measured Friedel pairs were merged as equivalent data.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

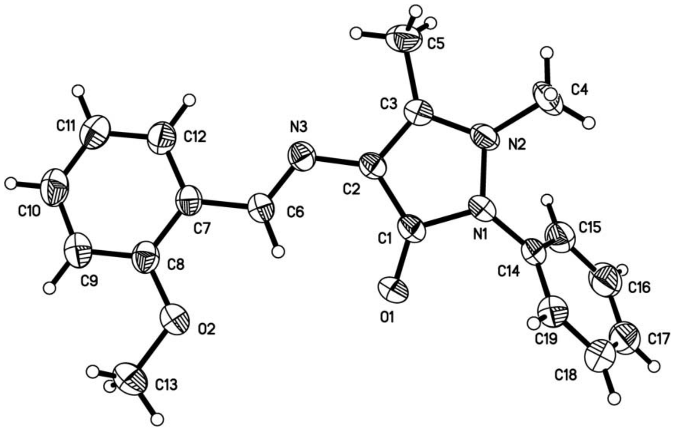

Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level for non-H atoms.

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