(E)-3-[(1,5-Dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-ylimino)methylene]phenyl 4-methylbenzenesulfonate

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In the title compound, $C_{25}H_{23}N_3O_4S$, the central benzene ring makes dihedral angles of 8.73 (3), 68.16 (7) and 41.67 (7)° with the pyrazolone ring, the sulfur-bound benzene ring and the phenyl ring, respectively. The crystal packing is stabilized by a weak non-classical intermolecular C—H⋯O=C hydrogen bond that forms a centrosymmetric dimer.

Comment

Schiff base ligands have received considerable attention in biology and chemistry (Kahwa *et al.*, 1986). Many Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics (Santos *et al.*, 2001). Among a large number of compounds, 4-amino-1,5-dimethyl-2-phenyl-pyrazol-3-one forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures of some of them, such as (*E*)-1,5-dimethyl-4-{2-[2-(2-nitrophenoxy)-ethoxy]benzyl-ideneamino}-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Diao & Chen, 2006) and (*E*)-4-[4-(4-chlorobenzyloxy)benzylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Hu, 2006) have been reported. Structural investigations may provide useful information concerning the coordination properties of Schiff bases functioning as ligands. We report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).

(I)
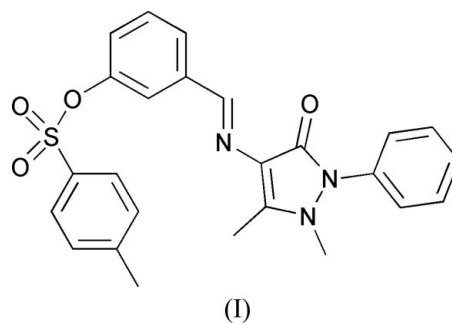
The bond lengths and angles of (I) are within normal ranges (Allen *et al.*, 1987). The pyrazolone ring (C16–C18/N1/N2/N3/O4) is almost planar, with an r.m.s. deviation for fitted atoms of 0.0369 Å. It makes a dihedral angle of 48.81 (6)° with the attached phenyl ring (C20–C25). The central benzene ring (C8–C14/O3) is nearly planar, with an r.m.s. deviation for fitted atoms of 0.0308 Å. This group makes dihedral angles of 8.73 (3), 68.16 (7) and 41.67 (7)° with the the pyrazolone ring, the sulfur-bound benzene ring (C1–C6) and the phenyl ring, respectively.

The crystal packing of (I) is stabilized by a weak non-classical intermolecular C—H⋯O=C hydrogen bond (Table 1) that forms a centrosymmetric dimer (Fig. 2).
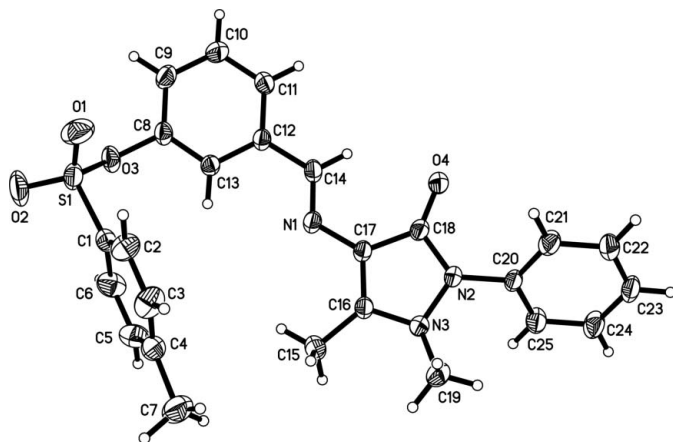
Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

Figure 2
A partial packing diagram of (I), viewed along the *b* axis, showing C—H⋯O hydrogen bonds (dashed lines).

Experimental

An anhydrous ethanol solution (50 ml) of 3-formylphenyl 4-methyl-benzenesulfonate (2.76 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) and the mixture was stirred at 350 K for 3 h under N_2, giving a yellow precipitate. The product was isolated, recrystallized from acetonitrile and dried in a vacuum to give pure (I) in 85% yield. Yellow single crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of an acetonitrile solution.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C11—H11⋯O4[i]	0.93	2.43	3.227 (3)	143

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

H atoms were included in calculated positions, with C—H = 0.93–0.96 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Crystal data

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