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(*E*)-2-{2-[(1,5-Dimethyl-3-oxo-1-phenyl-2,3-dihydro-1*H*-pyrazol-4-ylimino)methyl]-phenoxy}ethyl *p*-toluenesulfonate

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Key indicators

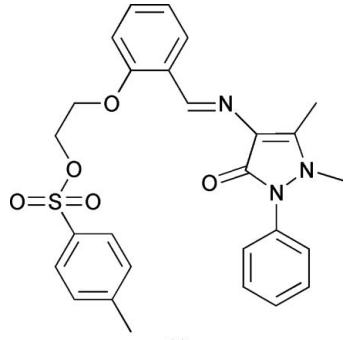
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.134
Data-to-parameter ratio = 15.5

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

In the title compound, $C_{27}H_{27}N_3O_5S$, the salicylaldehyde group makes dihedral angles of 20.47 (8), 43.28 (7) and 62.56 (7)° with the pyrazolone ring, the methyl-substituted benzene ring and the phenyl ring, respectively.

Comment

The synthesis and structures of Schiff bases have attracted much attention in biology and chemistry (Kahwa *et al.*, 1986; Klayman *et al.*, 1979). Many Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics (Santos *et al.*, 2001). Among the large number of compounds, 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures of some of these, such as (*E*)-4-[4-(4-chlorobenzyloxy)benzylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Hu, 2006), have been reported. We report here the synthesis and molecular structure of the title Schiff base compound, (I).



(I)

In the title molecule (Fig. 1), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The pyrazolone ring (C17–C19/N1–N3/O5) is almost planar, with an r.m.s. deviation for fitted atoms of 0.0310 Å. It makes a dihedral angle of 45.42 (7)° with its attached phenyl ring (C22–C27). The salicylaldehyde group (C10–C16/O4) is nearly planar, with an r.m.s. deviation for fitted atoms of 0.0297 Å. This group makes dihedral angles of 20.47 (8), 43.28 (7) and 62.56 (7)°, respectively, with the pyrazolone ring (C17–C19/N1–N3/O5), the C2–C7 benzene ring and the terminal C22–C27 phenyl ring.

Experimental

An anhydrous ethanol solution (50 ml) of 2-(2-formylphenoxy)ethyl-4-methylbenzenesulfonate (3.20 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 then dried in a vacuum to give pure compound (I) in 87% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{27}H_{27}N_3O_5S$	$Z = 4$
$M_r = 505.59$	$D_x = 1.344$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 12.505$ (2) Å	$\mu = 0.17$ mm^{-1}
$b = 25.713$ (4) Å	$T = 294$ (2) K
$c = 8.1019$ (14) Å	Block, yellow
$\beta = 106.453$ (3)°	0.36 × 0.30 × 0.20 mm
$V = 2498.4$ (7) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	13959 measured reflections
	5072 independent reflections
φ and ω scans	2744 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.040$
	$\theta_{max} = 26.4°$
$T_{min} = 0.921$, $T_{max} = 0.966$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.3756P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	
$wR(F^2) = 0.134$	
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.002$
5072 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
328 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
H-atom parameters constrained	

The H atoms were included in calculated positions and refined using a riding-model approximation [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2—H; C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene; C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl].

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*.

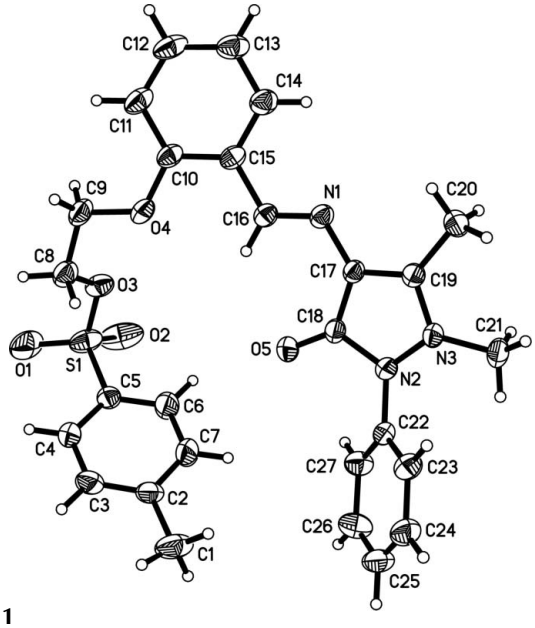


Figure 1
The structure of (I) showing the atom-labelling scheme, with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

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