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

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Key indicators

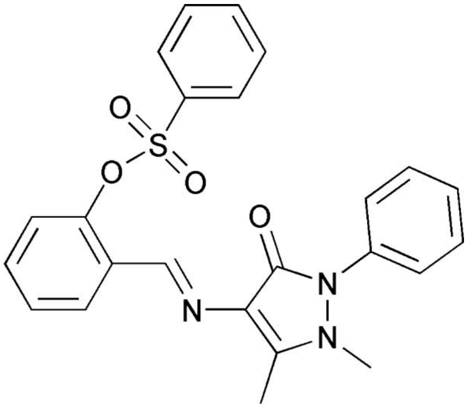
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.008 Å
R factor = 0.045
wR factor = 0.110
Data-to-parameter ratio = 7.2

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

In the title compound, $C_{24}H_{21}N_3O_4S$, the salicylaldehyde group makes dihedral angles of 2.81 (15), 26.11 (13) and 55.81 (14)°, respectively, with the pyrazolone ring, the phenyl ring attached to S and the phenyl ring attached to N. The crystal packing is stabilized by weak nonclassical intra- and intermolecular C—H···O hydrogen bonds and C—H···π interactions.

Comment

Schiff base ligands have received a good deal of 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 syntheses and crystal structures of some of them, such as (*E*)-1,5-dimethyl-4-{2-[2-(2-nitrophenoxy)ethoxy]benzylideneamino}-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 information is useful when investigating the coordination properties of Schiff bases functioning as ligands. We report here the synthesis and molecular structure of the title Schiff base compound, (I) (Fig. 1).



(I)

In the molecule of (I) (Fig. 1), bond lengths are within normal ranges (Allen *et al.*, 1987). The pyrazolone ring (C14–C16/N1/N2/N3/O4) is almost planar, with an r.m.s. deviation for fitted atoms of 0.0346 Å. It makes a dihedral angle of 58.02 (13)° with the attached phenyl ring (C19–C24). The salicylaldehyde group (C7–C13/O3) is essentially planar, with an r.m.s. deviation for fitted atoms of 0.0184 Å. This group

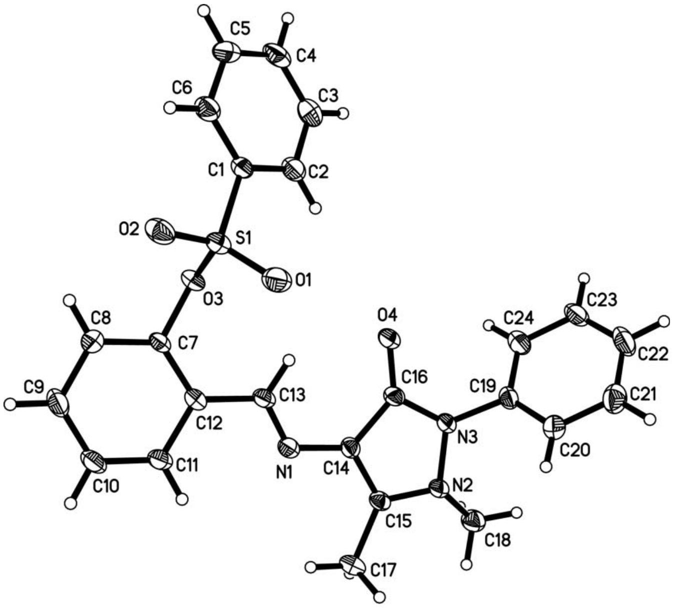


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

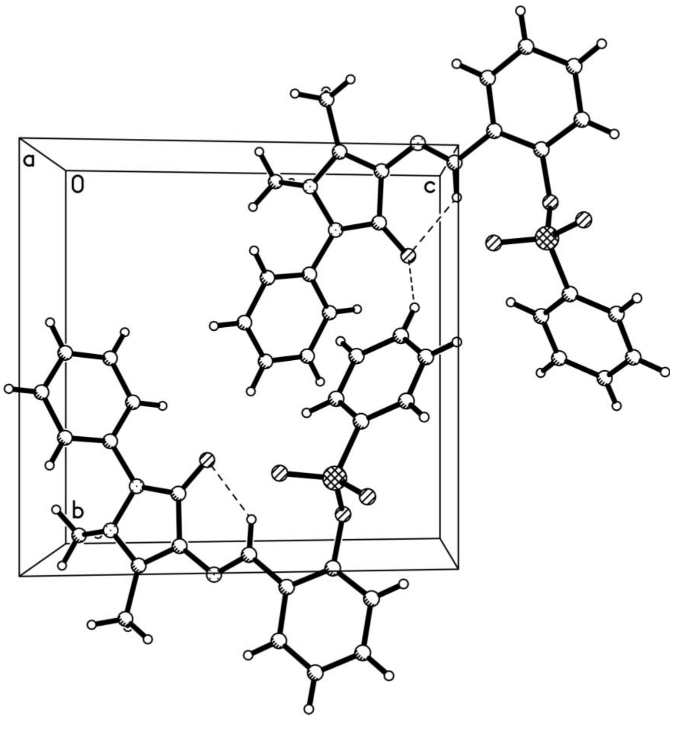


Figure 2
A partial packing diagram for (I), with hydrogen-bonding interactions drawn as dashed lines.

makes dihedral angles of 2.81 (15), 26.11 (13) and 55.81 (13)°, respectively, with the pyrazolone ring (C14–C16/N1/N2/N3/O4), the phenyl ring attached to S and the phenyl ring attached to N.

The crystal packing of (I) is stabilized by weak nonclassical intermolecular C—H···O hydrogen bonds, which link the molecules into infinite networks (Table 1, Fig. 2). An intramolecular C13—H13···O4=C16 hydrogen bond is found in (I), which helps to stabilize the conformation of the molecule. Furthermore, a weak C—H···π interaction is apparent (Table 1).

Experimental

An anhydrous ethanol solution (50 ml) of 2-formylphenyl benzenesulfonate (2.62 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 compound (I) in 85% yield. Yellow single crystals of (I) suitable for X-ray crystallographic analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{24}H_{21}N_3O_4S$
M_r = 447.51
Monoclinic, *Pc*
a = 8.822 (7) Å
b = 10.793 (8) Å
c = 11.029 (8) Å
β = 98.896 (13)°
V = 1037.5 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.941, $T_{\max}$ = 0.969
4141 measured reflections
2092 independent reflections
1621 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.110
S = 1.02
2092 reflections
292 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.23 e Å^{-3}
$\Delta\rho_{\min}$ = −0.43 e Å^{-3}
Absolute structure: Flack (1983), with 256 Friedel pairs
Flack parameter: 0.5 (2)

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

Cg is the centroid of the C19—C24 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O4	0.93	2.37	3.032 (6)	128
C4—H4···O4$^{\rm i}$	0.93	2.49	3.286 (7)	144
C17—H17*C*···O2$^{\rm ii}$	0.96	2.44	3.276 (7)	145
C3—H3···*Cg*$^{\rm i}$	0.93	2.60	3.516 (2)	168

Symmetry codes: (i) $x, -y+1, z+\frac{1}{2}$; (ii) $x-1, -y, z-\frac{1}{2}$.

H atoms were included in calculated positions and refined using a riding-model approximation, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for Csp^2 H, and C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl H. The Flack parameter (Flack, 1983) indicates probable inversion twinning, but has a high standard uncertainty.

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*.

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