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4-{(*E*)-[2-(4-Iodobutoxy)benzylidene]amino}-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

Hoong-Kun Fun,[a]*‡ Madhukar Hemamalini,[a] Abdullah M. Asiri[b]§ and Salman A. Khan[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Department of Chemistry, Faculty of Science, King Abdu Aziz University, Jeddah, Saudi Arabia
Correspondence e-mail: hkfun@usm.my

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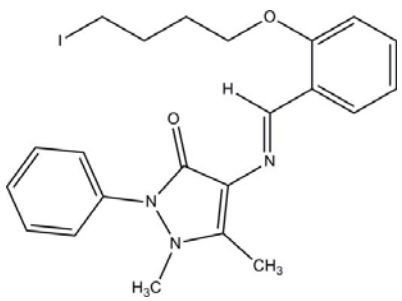
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.159; data-to-parameter ratio = 37.8.

The title Schiff base compound, $C_{22}H_{24}IN_3O_2$, adopts an E configuration about the central C=N bond. The pyrazolone ring makes a dihedral angle of 49.68 (10)° with its attached phenyl ring. The phenolate plane makes dihedral angles of 16.78 (9) and 50.54 (9)°, respectively, with the pyrazolone ring and the terminal phenyl ring. An intramolecular C—H···O hydrogen bond generates an S(6) ring motif. In the crystal structure, an intermolecular C—H···O hydrogen bond is also observed.

Related literature

For background to and applications of Schiff bases, see: Tarafder *et al.* (2002); Silver & Soderlund (2005); Vicini *et al.* (2003); Ozdemir *et al.* (2007); Joshi *et al.* (2004). For background to and the biological activity of 4-aminoantipyrene and its derivatives, see: Jain *et al.* (2003); Filho *et al.* (1998); Sondhi *et al.* (1999); Mishra (1999); Sondhi *et al.* (2001). For related structures, see: Eryigit & Kendi (1998); Manikandan *et al.* (2000). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{22}H_{24}IN_3O_2$
M_r = 489.34
Monoclinic, $P2_1/c$
a = 11.5235 (10) Å
b = 16.4156 (14) Å
c = 11.2828 (9) Å
β = 94.010 (2)°
V = 2129.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.53 mm^{-1}
T = 100 K
0.41 × 0.34 × 0.29 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.571, T_{max} = 0.663
36214 measured reflections
9632 independent reflections
7935 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.159
S = 1.05
9632 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.26 e Å^{-3}
$\Delta\rho_{min}$ = −1.68 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O1	0.93	2.30	2.995 (2)	132
C17—H17B···O1^{i}	0.97	2.42	3.193 (2)	137

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2554).

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§ On secondment to: The Center of Excellence for Advanced Materials Research, King Abdu Aziz University, Jeddah 21589, Saudi Arabia.