Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Abdullah M. Asiri,[a] Salman A. Khan,[a] Kong Wai Tan[b] and Seik Weng Ng[b]*

[a]Chemistry Department, Faculty of Science, King Abdul Aziz University, PO Box 80203, Jeddah 21589, Saudi Arabia, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

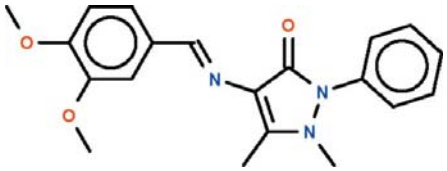
Received 15 June 2010; accepted 16 June 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.103; data-to-parameter ratio = 17.4.

The imino–carbon double-bond in the title Schiff base, $C_{20}H_{21}N_3O_3$, has an E configuration; the six-membered aromatic substituent (r.m.s. deviation = 0.012 Å) is nearly coplanar with five-membered pyrazole substituent (r.m.s. deviation = 0.031 Å), the dihedral angle between the two systems being 11.4 (1)°]. The phenyl ring connected to the pyrazole ring is aligned at 45.5 (1)° with respect to this five-membered ring. The N atoms in the ring show pyramidal coordinations.

Related literature

For background literature on Schiff bases derived from 4-aminoantipyridine, see: Montalvo-González & Ariza-Castolo (2003).



Experimental

Crystal data

$C_{20}H_{21}N_3O_3$
M_r = 351.40
Monoclinic, $P2_1/c$
a = 12.5584 (8) Å
b = 10.4752 (7) Å
c = 14.6002 (9) Å
β = 109.039 (1)°
V = 1815.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.35 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
16900 measured reflections
4164 independent reflections
3442 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.103
S = 1.00
4164 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdul Aziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2733).

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