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4-[(Anthracen-9-ylmethylidene)amino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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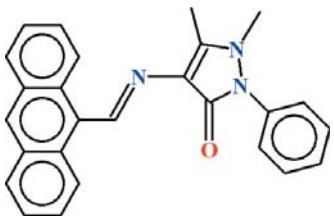
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.109; data-to-parameter ratio = 13.2.

In the title compound, $C_{26}H_{21}N_3O$, the phenyl ring of the 4-aminoantipyrine group and the heterocyclic five-membered ring along with its substituents, except for the N-bound methyl group (r.m.s. deviation = 0.0027 Å), form a dihedral angle of 54.20 (5)°. Two S(6) ring motifs are formed due to intramolecular C—H···N and C—H···O hydrogen bonds. In the crystal, molecules are linked into supramolecular chains along the a-axis direction *via* C—H···O contacts.

Related literature

For background to pyrazol-3-ones, see: Asiri & Khan (2010); Crane *et al.* (1985); Desai *et al.* (2010); Rai *et al.* (2009); Takagi *et al.* (1987); Yao *et al.* (2007); Zhang *et al.* (2005); For related crystal structures, see: Li & Zhang (2006). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{26}H_{21}N_3O$
M_r = 391.46
Monoclinic, $P2_1/n$
a = 7.6603 (3) Å
b = 16.4549 (6) Å
c = 15.8849 (6) Å
β = 95.243 (1)°
V = 1993.91 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.32 × 0.24 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.975, T_{max} = 0.980
14673 measured reflections
3593 independent reflections
2791 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
S = 1.06
3593 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5a···O1^{i}	0.96	2.59	3.530 (2)	167
C5—H5c···O1^{ii}	0.96	2.57	3.5305 (19)	177
C12—H12···O1	0.93	2.37	3.0375 (19)	128
C15—H15···N1	0.93	2.42	3.024 (2)	123

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x+1, y, z$.

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: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2768).

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