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2-[(3,5-Dimethyl-1-phenyl-1*H*-pyrazol-4-yl)methylidene]indan-1,3-dione

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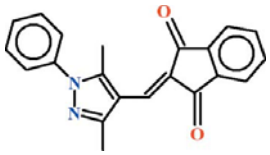
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.112; data-to-parameter ratio = 13.0.

In the title compound, $C_{21}H_{16}N_2O_2$, the five-membered heterocyclic ring makes a dihedral angle of 47.06 (6)° with the attached benzene ring, whereas the indan-1,3-dione ring system and the benzene ring are oriented at a dihedral angle of 21.92 (7)°. In the crystal, inversion dimers linked by pairs of C—H···O hydrogen bonds generate $R_2^2(22)$ loops. Aromatic π–π stacking interactions [centroid–centroid distances = 3.8325 (12)–3.8600 (12) Å] also occur.

Related literature

For background to donor–acceptor chromophores, see: Asiri *et al.* (2006); Asiri & Khan (2009); Koyuncu *et al.* (2010); Kulhanek *et al.* (2011); Wang *et al.* (2011). For related structures, see: Belyakov *et al.* (2008); Fun *et al.* (2010). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{21}H_{16}N_2O_2$
M_r = 328.36
Monoclinic, $C2/c$
a = 14.6655 (3) Å
b = 7.8902 (2) Å
c = 28.6651 (7) Å
β = 98.251 (1)°
V = 3282.61 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.26 × 0.23 × 0.21 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.975, T_{max} = 0.985
12302 measured reflections
2970 independent reflections
2106 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
S = 1.01
2970 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 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
C18—H18···O1^{i}	0.93	2.58	3.377 (3)	145

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

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: HB6509).

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