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(*E*)-2-Methyl-6-[(1-phenyl-1*H*-pyrazol-4-yl)methylidene]cyclohexanone

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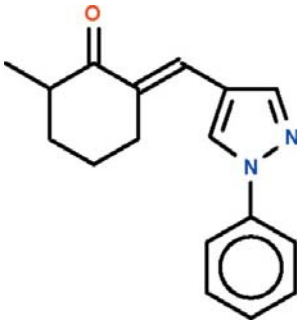
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.062; wR factor = 0.172; data-to-parameter ratio = 12.0.

The asymmetric unit of the title compound, $C_{17}H_{18}N_2O$, contains two independent molecules. In both, the cyclohexane ring adopts a flattened chair conformation, and the 3- and 4-methylene C atoms as well as the methyl C atoms are disordered over two positions, the occupancy of the major component being 68 (1)% in one molecule and 64 (1)% in the other. The phenyl and pyrazole rings in both molecules are approximately coplanar, the r.m.s. deviations being 0.048 and 0.015 Å, respectively. Weak intermolecular C—H···O hydrogen bonding is present in the crystal structure.

Related literature

For a recent report on similar heterocylic compounds derived from substituted 1-phenylpyrazole-4-carboxaldehydes>, see: Asiri & Khan (2010).



Experimental

Crystal data

$C_{17}H_{18}N_2O$
M_r = 266.33
Triclinic, $P\overline{1}$
a = 6.1152 (8) Å
b = 10.3757 (13) Å
c = 22.734 (3) Å
α = 77.542 (2)°
β = 89.667 (2)°
γ = 78.510 (2)°
V = 1379.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.20 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
14492 measured reflections
4890 independent reflections
3235 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.172
S = 1.03
4890 reflections
408 parameters
47 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O1^{i}	0.95	2.29	3.157 (4)	152
C26—H26···O2^{ii}	0.95	2.30	3.224 (4)	164
C30—H30···O2^{ii}	0.95	2.57	3.506 (4)	167

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

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5225).

References

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