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2-(Dipropylamino)-4-[(4-methoxyphenyl)-methylene]-1-phenyl-1*H*-imidazol-5(4*H*)-one

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.058
wR factor = 0.164
Data-to-parameter ratio = 18.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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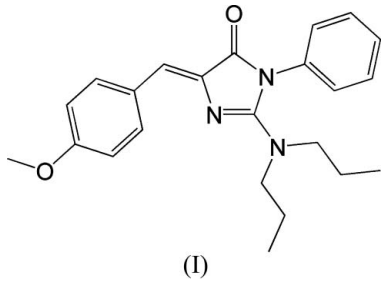
In the title compound, $C_{23}H_{27}N_3O_2$, the packing of the molecules in the crystal structure appears to be influenced by C—H···O hydrogen-bonding interactions.

Comment

Imidazolinones are important heterocyclic compounds possessing remarkable biological activities (Hu *et al.*, 2004). Many derivatives of imidazolinone have been prepared and their biological activities studied in recent years (Ding *et al.*, 2004). As part of our ongoing studies in this area, we obtained the title compound, (I) (Fig. 1), which may be used as a new precursor for obtaining bioactive molecules. Its crystal structure is presented here.



(I)

The five-membered imidazolone ring (N1/N2/C9/C10/C17) in (I) is planar. Phenyl ring C11–C16 is twisted with respect to the imidazolone ring, making a dihedral angle of 57.5 (2)°. One of the dipropylamino alkyl side chains (C21—C22—C23) is disordered over two positions. As well as a possible intramolecular C—H···N interaction, there are intermolecular C—H···O bonds (Table 1) which may help to stabilize the crystal packing (Fig. 2).

Experimental

Phenyl isocyanate (3 mmol) was added to a solution of iminophosphorane (1.44 g, 3 mmol) in dry dichloromethane (15 ml) under nitrogen at room temperature. After standing for 6 h at room temperature, the solvent was removed under reduced pressure and diethyl ether/petroleum ether (1:2, 20 ml) was added to precipitate triphenylphosphine oxide. After filtration, the solvent was removed to give the carbodiimide, which was used directly without further purification. To a solution of the carbodiimide prepared above in dichloromethane (15 ml) was added dipropylamine (3 mmol). After the reaction mixture had been allowed to stand for 6 h, the solution was concentrated under reduced pressure and the residue was recrystallized from dichloromethane/petroleum ether (1:4) to give the title compound in 80% yield (m.p. 438 K). Suitable crystals of (I) were obtained by vapour diffusion of ethanol into a solution in dichloromethane at room temperature.

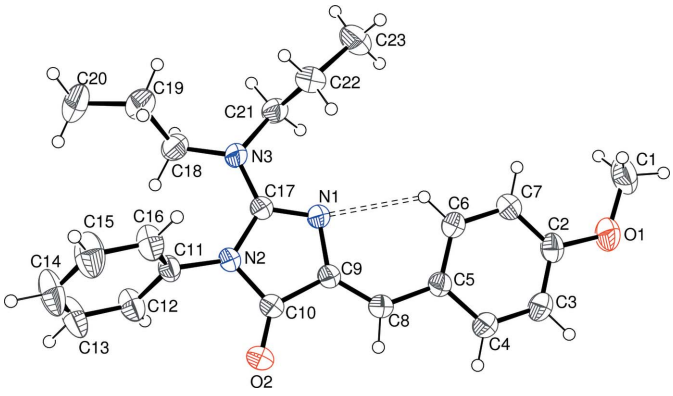


Figure 1
View of (I), with displacement ellipsoids drawn at the 40% probability level. H atoms are represented by spheres of arbitrary size. Only the major disorder component of the C21/C22/C23 chain is shown. The possible C—H···N interaction is shown as a dashed line.

Crystal data

$C_{23}H_{27}N_3O_2$
M_r = 377.48
Orthorhombic, *Pbca*
a = 8.2388 (7) Å
b = 19.9018 (17) Å
c = 25.697 (2) Å
V = 4213.4 (6) Å^3
Z = 8
D_x = 1.190 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 292 (2) K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.977, T_{max} = 0.992
40947 measured reflections
5130 independent reflections
3292 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.164
S = 1.02
5130 reflections
285 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0891P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O2^{i}	0.93	2.48	3.361 (2)	159
C6—H6···N1	0.93	2.43	3.074 (2)	126
C1—H1A···O1^{ii}	0.96	2.55	3.493 (3)	168

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

The C21/C22/C23 fragment (and attached H atoms) is disordered over two positions in a 0.677 (5):0.323 (5) population ratio (sum constrained to unity). H atoms were placed at calculated positions (C—H = 0.93–0.98 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

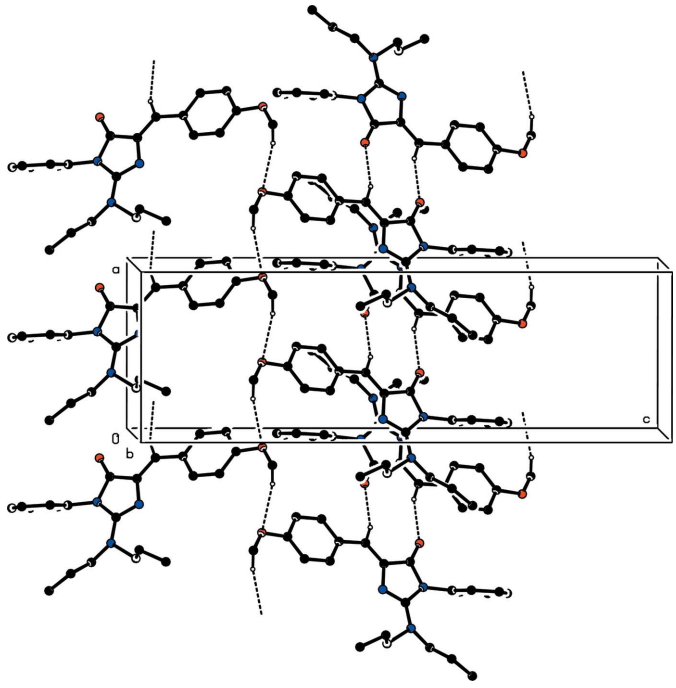


Figure 2
Packing diagram of (I), showing the C—H···O associations (dashed lines). H atoms not involved in these interactions have been omitted.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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