organic papers

2-Diethylamino-3-phenylquinazolin-4(3*H*)-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.052
wR factor = 0.136
Data-to-parameter ratio = 17.4

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

In the title compound, $C_{18}H_{19}N_3O$, the quinazoline system is approximately planar. The plane of the substituent phenyl ring forms a dihedral angle of 63.9 (2)° with respect to the mean plane of the quinazolinone ring system.

Comment

Quinazolinones are important heterocyclic compounds which exhibit good biological and pharmaceutical activity, including anti-inflammatory, antifungal, anticancer and AMPA-receptor antagonistic properties (Shiba *et al.*, 1997). As part of our work on the preparation of potentially active heterocycles (Ding *et al.*, 2000), we have obtained the title compound, (I).

(I)
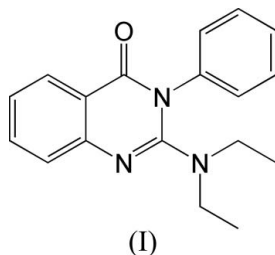
In (I), the quinazoline system is approximately planar (Fig. 1). The plane of the phenyl ring bound to N2 forms a dihedral angle of 63.9 (2)° with respect to the mean plane of the quinazolinone ring system, and the N2—C13 bond is twisted out of the quinazolinone plane [C14—C13—N2—C8 torsion angle = −60.28 (19)°]. The C8—N3, C8—N2, C13—N2 and C7—N2 bond lengths [1.3677 (18), 1.4072 (17), 1.4499 (18) and 1.4139 (19) Å, respectively] indicate some degree of delocalization around the heterocyclic six-membered ring (Yuan & Ding, 2006).

Experimental

Phenyl isocyanate (0.36 g, 3 mmol) was added to a solution of *N*-(2-ethoxycarbonylphenyl)iminophosphorane (1.45 g, 3 mmol) in anhydrous dichloromethane (15 ml) under dry nitrogen at room temperature. The reaction mixture was left unstirred for 8 h at room temperature and the solvent was then removed under reduced pressure and diethyl ether–petroleum ether (1:2 *v/v*, 20 ml) was added to precipitate triphenylphosphine oxide. After filtration, a solution of the carbodiimide was added to a solution of diethylamine in anhydrous dichloromethane (5 ml). After stirring the reaction mixture for 8 h, the solvent was removed under reduced pressure and the residue was recrystallized from ethanol to give the title compound (yield 88%; m.p. 388 K). Single crystals suitable for X-ray diffraction were obtained by recrystallization from a hexane–dichloromethane (1:3 *v/v*) solution at room temperature.
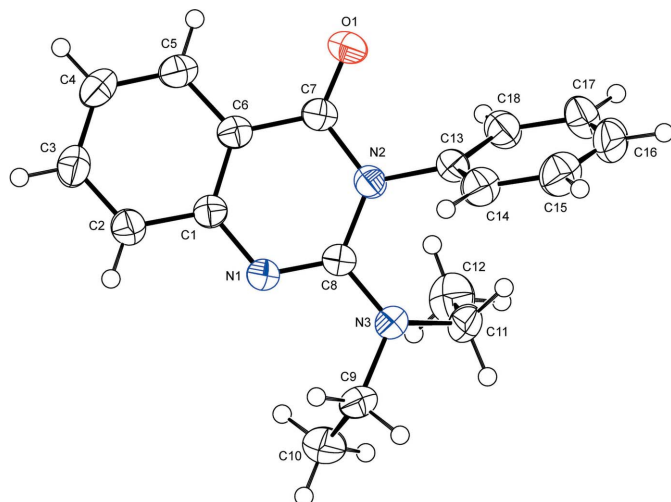
Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

Crystal data

$C_{18}H_{19}N_3O$
$M_r = 293.36$
Orthorhombic, $Pbca$
$a = 8.4259\ (7)$ Å
$b = 10.9029\ (9)$ Å
$c = 33.263\ (3)$ Å
$V = 3055.7\ (4)$ Å^3

$Z = 8$
$D_x = 1.275$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 298\ (2)$ K
Block, white
$0.30 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.976$, $T_{max} = 0.992$

17133 measured reflections
3493 independent reflections
2931 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.136$
$S = 1.05$
3493 reflections
201 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0701P)^2 + 0.7969P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

H atoms were placed at calculated positions, with C—H = 0.93, 0.96 and 0.97 Å for aromatic, methylene and methyl H atoms, respectively. They were refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for the methyl groups. The methyl groups were allowed to rotate about their local threefold axes.

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

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