5-Benzoyl-1-*n*-butyl-4-phenylpyrimidin-2(1*H*)-one

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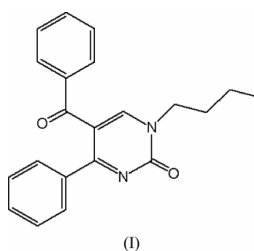
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Key indicators

Single-crystal X-ray study
$T = 293$ K
Mean σ(C–C) = 0.005 Å
R factor = 0.062
wR factor = 0.197
Data-to-parameter ratio = 15.4

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

The title compound, $C_{21}H_{20}N_2O_2$, crystallizes in the monoclinic space group $P2_1/c$. The pyrimidine ring is essentially planar. The structure is stabilized by intermolecular C—H···O interactions.

Comment

For biological and medicinal reasons, pyrimidines have attracted much attention, and their chemistry has been investigated extensively (Brown, 1984, 1985). In particular, various analogues of pyrimidines possess effective antibacterial, antifungal, antiviral, anti-AIDS, insecticidal and miticidal activity (De Clerq & Walker, 1985). In this paper, we report the structure of the title compound, (I), a pyrimidine derivative. The crystal structure of (I) confirms the molecular formula based on NMR and IR spectroscopic data.

(I)

The pyrimidine ring is essentially planar, with a maximum deviation of 0.050 (3) Å for atom C4. The dihedral angle between the two phenyl rings [*A* (C10–C15) and *B* (C16–C21)] is 88.7 (1)°, and the pyrimidine ring forms dihedral angles of 117.1 (1) and 131.7 (1)° with rings *A* and *B*, respectively. All the geometric parameters of (I) (Table 1) are in good agreement with those in related structures (Öztürk *et al.*, 1997, 1999; Akkurt *et al.*, 1992, 2003; Özbey *et al.*, 1991; Akkurt & Hiller, 1993). It is interesting to note the relative orientation of the *n*-butyl group attached to the pyrimidine ring. The least-squares plane through atoms N2, C5, C6, C7 and C8 is almostly perpendicular to the pyrimidine ring, with a dihedral angle of 91.3 (2)°. The intermolecular interactions, which stabilize the crystal structure, are given in Table 2.

Experimental

An equimolar mixture of 4-benzoyl-5-phenyl-2,3-furandione (0.50 g, 180 mmol) and *n*-butylurea (0.21 g, 180 mmol) was refluxed in boiling benzene for 4.5 h. The solvent was evaporated and the remaining oily residue was treated with dry ether to give a white precipitate, which was filtered off and recrystallized from *n*-butanol (yield 0.45 g, 76%) (Altural *et al.*, 1989). The melting point was determined on an Electrothermal 9200 apparatus and is uncorrected. Microanalysis was performed on a Carlo–Erba Elemental Analyser Model 1108. The IR spectrum was recorded on a Perkin–Elmer 421 spectrometer using

potassium bromide pellets. The ^{1}H NMR spectrum was obtained on a Varian EM 360 L spectrometer with TMS as an internal standard. M.p. 466 K. IR (KBr, cm^{-1}): ν 3050–2860 (aromatic and aliphatic C—H), 1670 (s, broad C=O), 1590, 1575, 1520, 1500, 1460 (C=C, aromatic rings); ^{1}H NMR (CDCl$_3$): δ 8.2 (s, 1H at C-6), 7.8–7.1 (m, 10H, Ph—H), 4.0 (t, 2H, N-CH$_2$), 2.1–1.1 (m, 4H, 2 × CH$_2$), 1.0 (t, 3H, CH$_3$). Analysis calculated for C$_{21}$H$_{20}$N$_2$O$_2$: C 75.88, H 6.06, N 8.43%; found: C 76.06, H 5.90, N 8.30%.

Crystal data

C$_{21}$H$_{20}$N$_2$O$_2$	$D_x = 1.239$ Mg m^{-3}
$M_r = 332.39$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 15
$a = 10.125$ (5) Å	reflections
$b = 15.518$ (5) Å	$\theta = 25\text{--}35°$
$c = 11.398$ (5) Å	$\mu = 0.08$ mm^{-1}
$\beta = 95.727$ (5)°	$T = 293$ (2) K
$V = 1781.9$ (13) Å^3	Prism, white
$Z = 4$	$0.42 \times 0.42 \times 0.33$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer	1865 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$\theta_{max} = 26.3°$
Absorption correction: refined from ΔF (Parkin $et~al.$, 1995; cubic fit to sinθ/λ, 24 parameters)	$h = -12 \rightarrow 12$
	$k = 0 \rightarrow 19$
	$l = 0 \rightarrow 14$
$T_{min} = 0.967$, $T_{max} = 0.974$	3 standard reflections
3491 measured reflections	frequency: 120 min
3491 independent reflections	intensity decay: 2%

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.1151P)^2]$
$wR(F^2) = 0.197$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
3491 reflections	$\Delta\rho_{max} = 0.47$ e Å^{-3}
226 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.223 (3)	N2—C1	1.336 (3)
O2—C9	1.219 (3)	N2—C4	1.401 (3)
N1—C3	1.310 (3)	N2—C5	1.472 (4)
N1—C4	1.373 (4)		
C3—N1—C4	120.4 (2)	O1—C4—N1	123.0 (2)
C1—N2—C4	120.9 (2)	O1—C4—N2	119.1 (2)
C1—N2—C5	120.6 (2)	N1—C4—N2	117.9 (2)
C4—N2—C5	118.5 (2)	N2—C5—C6	113.5 (3)
N2—C1—C2	122.1 (2)	O2—C9—C2	119.8 (2)
N1—C3—C2	122.6 (2)	O2—C9—C10	119.6 (2)
N1—C3—C16	115.2 (2)		
C1—N2—C5—C6	89.8 (4)	N2—C5—C6—C7	−171.5 (4)
C4—N2—C5—C6	−86.6 (4)	C5—C6—C7—C8	178.1 (6)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C1—H1⋯O1^i	0.93	2.42	3.236 (4)	147
C5—H5A⋯O1^i	0.97	2.34	3.199 (4)	148

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

All H atoms were placed in idealized positions and treated as riding, with C—H distances of 0.93 or 0.97 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl group and 1.2U_{eq}(C) for all other H atoms. The C7—C8 bond length was restrained to 1.54 (3) Å.
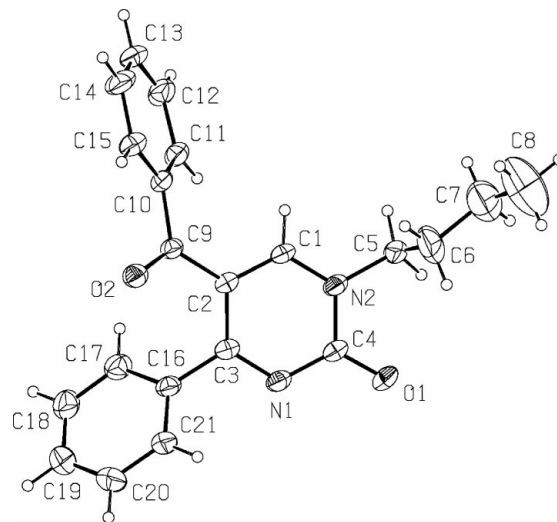

Figure 1
An $ORTEP$-3 (Farrugia, 1997) drawing of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

Data collection: CAD-4 $EXPRESS$ (Enraf–Nonius, 1994); cell refinement: CAD-4 $EXPRESS$; data reduction: $XCAD$4 (Harms & Wocadlo, 1995); program(s) used to solve structure: SIR97 (Altomare $et~al.$, 1999); program(s) used to refine structure: $SHELXL$97 (Sheldrick, 1997); molecular graphics: $ORTEP$-3 $for~Windows$ (Farrugia, 1997); software used to prepare material for publication: $PARST$ (Nardelli, 1995) and $WinGX$ (Farrugia, 1999).

References

Akkurt, M., Güldeste, A., Soylu, H., Altural, B. & Sarıpınar, E. (1992). $Acta~Cryst.$ C**48**, 315–317.
Akkurt, M. & Hiller, W. (1993). $Acta~Cryst.$ C**49**, 747–749.
Akkurt, M., Sarıpınar, E., Öztürk, S., Yılmaz, Ç. & Fun, H.-K. (2003). $Z.~Kristallogr.$ **218**, 488–491.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). $J.~Appl.~Cryst.$ **32**, 115–119.
Altural, B., Akçamur, Y., Sarıpınar, E., Yıldırım, İ. & Kollenz, G. (1989). $Monatsh.~Chem.$ **120**, 1015–1020.
Brown, D. J. (1984). $Compr.~Heterocycl.~Chem.$ **3**, 57–61.
Brown, D. J. (1985). $The~Chemistry~of~Heterocyclic~Compounds,~The~Pyrimidines$, Suppl. II, edited by A. Weissberger & E. C. Taylor. New York: Interscience.
De Clerq, E. & Walker, R. T. (1985). $Pharm.~Ther.$ **26**, 1–44.
Enraf–Nonius (1994). CAD-4 $EXPRESS$. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). $J.~Appl.~Cryst.$ **30**, 565.
Farrugia, L. J. (1999). $J.~Appl.~Cryst.$ **32**, 837–838.
Harms, K. & Wocadlo, S. (1995). $XCAD$4. University of Marburg, Germany.
Nardelli, M. (1995). $J.~Appl.~Cryst.$ **28**, 659.
Özbey, S., Kendi, E., Akçamur, Y., Yıldırım, İ., Elerman, Y. & Soylu, H. (1991). $Acta~Cryst.$ C**47**, 1105–1106.
Öztürk, S., Akkurt, M., Hökelek, T. & Yıldırım, İ. (1997). $Cryst.~Res.~Technol.$ **32**, 585–589.
Öztürk, S., Akkurt, M., Razak, I. A., Fun, H. K. & Yıldırım, İ. (1999). $Acta~Cryst.$ C**55**, 97–99.
Parkin, S., Moezzi, B. & Hope, H. (1995). $J.~Appl.~Cryst.$ **28**, 53–56.
Sheldrick, G. M. (1997). $SHELXL$97. University of Göttingen, Germany.