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4-(4-Methoxyphenyl)-6-phenylpyrimidin-2-amine

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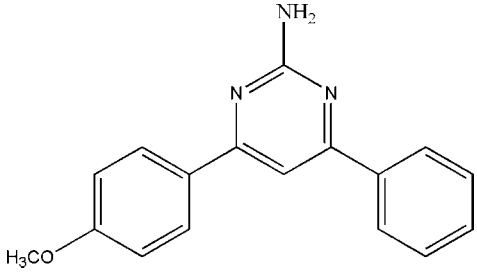
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.137; data-to-parameter ratio = 18.2.

The title compound, $C_{17}H_{15}N_3O$, was prepared by the reaction of 1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one and guanidine nitrate with ethanol at room temperature. The dihedral angles formed by the two benzene rings with the pyridine ring are 13.19 (1) and 6.39 (2)°. There are two weak intramolecular C—H···N as well as two weak intermolecular N—H···N hydrogen-bonding interactions in the crystal structure.

Related literature

For related literature, see: Arvanitis *et al.* (1999); Brown *et al.* (1988); Ligthart *et al.* (2005); Blatt (1951); Fun *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{15}N_3O$
M_r = 277.32
Monoclinic, $P2_1/c$
a = 12.590 (3) Å
b = 6.9590 (14) Å
c = 16.320 (3) Å
β = 96.61 (3)°
V = 1420.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.20 × 0.15 × 0.11 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
18765 measured reflections
3476 independent reflections
1939 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.137
S = 1.04
3476 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N2^{i}	0.86	2.18	3.012 (3)	163
N3—H3B···N1^{ii}	0.86	2.40	3.191 (3)	154
C6—H6A···N2	0.93	2.47	2.795 (3)	101
C17—H17A···N1	0.93	2.50	2.822 (3)	101

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2455).

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supplementary materials

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4-(4-Methoxyphenyl)-6-phenylpyrimidin-2-amine

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Comment

Functionalized pyrimidines play a major role in the synthesis of different drug molecules (Arvanitis *et al.*, 1999; Fun *et al.*,2006). They are important for the synthesis of pteridine- and purine-related compounds (Brown *et al.*,1988) and also for multiple hydrogen-bonding interactions in molecular recognition and supramolecular chemistry (Ligthart *et al.*, 2005). They have biochemical and pharmacological applications. The recent growing interest in them is also due to the ability. The title compound has been synthesized and we report here its crystal structure.

In the crystal structure (Fig. 1), the dihedral angles formed by the phenyl rings (C2–C7) and (C12–C17) with the plane through the pyridine ring are 13.19 (1) and 6.39 (2)°, respectively. The mean value of the C═N double bond lengths is 1.3458 (3) Å. Intramolecular C—H···N as well as intermolecular N—H···N hydrogen bonds are present in the crystal structure.

Experimental

A mixture of 1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one (Blatt, 1951) (0.02 mol) and guanidine (0.02 mol) was stirred with ethanol (50 ml) at 353 K for 4 h, affording the title compound (4.7 g, yield 85%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H = 0.86Å and C—H = 0.93 or 0.96 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq} of the parent atoms.

Figures

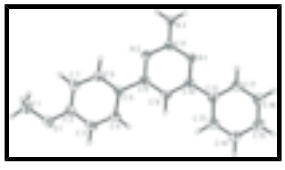


Fig. 1. The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

4-(4-Methoxyphenyl)-6-phenylpyrimidin-2-amine

Crystal data

$C_{17}H_{15}N_3O$	F_{000} = 584
M_r = 277.32	D_x = 1.297 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 156 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation

	λ = 0.71073 Å
a = 12.590 (3) Å	Cell parameters from 25 reflections
b = 6.9590 (14) Å	θ = 4–14º
c = 16.320 (3) Å	μ = 0.08 mm^{-1}
β = 96.61 (3)º	*T* = 295 (2) K
V = 1420.4 (5) $Å^3$	Block, yellow
Z = 4	0.20 × 0.15 × 0.11 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.047
Radiation source: fine-focus sealed tube	θ_{max} = 28.3º
Monochromator: graphite	θ_{min} = 1.6º
T = 295(2) K	*h* = −16→14
ω scans	*k* = −9→9
Absorption correction: none	*l* = −20→21
18765 measured reflections	3 standard reflections
3476 independent reflections	every 100 reflections
1939 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.0825P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.137	$(\Delta/\sigma)_{max} < 0.001$
S = 1.04	$\Delta\rho_{max}$ = 0.15 e $Å^{-3}$
3476 reflections	$\Delta\rho_{min}$ = −0.13 e $Å^{-3}$
191 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0094 (19)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.24387 (10)	−0.00893 (18)	0.60359 (8)	0.0734 (4)
N1	0.15472 (10)	0.95596 (17)	0.29535 (7)	0.0453 (3)
N2	0.09537 (10)	0.66067 (17)	0.35172 (7)	0.0453 (3)
N3	−0.00988 (10)	0.82471 (18)	0.25208 (8)	0.0561 (4)
H3A	−0.0218	0.9191	0.2183	0.067*
H3B	−0.0575	0.7368	0.2543	0.067*
C1	0.15845 (16)	−0.1366 (3)	0.61267 (12)	0.0743 (6)
H1B	0.1842	−0.2423	0.6473	0.111*
H1C	0.1298	−0.1843	0.5595	0.111*
H1D	0.1035	−0.0699	0.6374	0.111*
C2	0.22320 (14)	0.1531 (2)	0.55656 (9)	0.0540 (4)
C3	0.31007 (15)	0.2681 (3)	0.54745 (11)	0.0657 (5)
H3C	0.3768	0.2367	0.5747	0.079*
C4	0.29889 (14)	0.4287 (2)	0.49845 (11)	0.0598 (5)
H4A	0.3584	0.5048	0.4930	0.072*
C5	0.20075 (12)	0.4801 (2)	0.45685 (9)	0.0461 (4)
C6	0.11446 (14)	0.3651 (2)	0.46848 (10)	0.0577 (5)
H6A	0.0474	0.3974	0.4422	0.069*
C7	0.12464 (14)	0.2034 (2)	0.51802 (11)	0.0601 (5)
H7A	0.0649	0.1292	0.5251	0.072*
C8	0.18777 (12)	0.6494 (2)	0.40153 (9)	0.0448 (4)
C9	0.26531 (13)	0.7888 (2)	0.39975 (10)	0.0517 (4)
H9A	0.3288	0.7812	0.4349	0.062*
C10	0.24733 (12)	0.9407 (2)	0.34480 (9)	0.0440 (4)
C11	0.08306 (12)	0.8146 (2)	0.30137 (9)	0.0438 (4)
C12	0.32930 (12)	1.0912 (2)	0.33710 (9)	0.0469 (4)
C13	0.43102 (14)	1.0775 (3)	0.37899 (11)	0.0631 (5)
H13A	0.4484	0.9718	0.4127	0.076*
C14	0.50694 (15)	1.2166 (3)	0.37190 (12)	0.0703 (5)
H14A	0.5748	1.2038	0.4006	0.084*
C15	0.48324 (16)	1.3748 (3)	0.32253 (12)	0.0711 (5)
H15A	0.5343	1.4696	0.3180	0.085*
C16	0.38334 (15)	1.3903 (3)	0.28016 (12)	0.0734 (6)
H16A	0.3664	1.4964	0.2465	0.088*
C17	0.30746 (14)	1.2500 (3)	0.28692 (11)	0.0629 (5)
H17A	0.2402	1.2624	0.2571	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0769 (9)	0.0640 (8)	0.0746 (9)	−0.0011 (7)	−0.0118 (7)	0.0237 (7)
N1	0.0424 (8)	0.0410 (7)	0.0501 (7)	−0.0002 (6)	−0.0043 (6)	−0.0033 (6)
N2	0.0435 (8)	0.0395 (7)	0.0506 (7)	0.0027 (6)	−0.0052 (6)	−0.0008 (6)
N3	0.0473 (8)	0.0421 (8)	0.0731 (9)	−0.0043 (6)	−0.0176 (7)	0.0087 (6)

C1	0.0885 (15)	0.0595 (12)	0.0758 (13)	−0.0001 (11)	0.0140 (11)	0.0181 (10)
C2	0.0608 (12)	0.0501 (9)	0.0485 (9)	0.0030 (8)	−0.0046 (8)	0.0070 (7)
C3	0.0533 (11)	0.0670 (12)	0.0713 (12)	0.0035 (9)	−0.0170 (9)	0.0151 (9)
C4	0.0496 (11)	0.0578 (11)	0.0686 (11)	−0.0040 (8)	−0.0083 (9)	0.0097 (9)
C5	0.0455 (10)	0.0463 (9)	0.0443 (8)	0.0019 (7)	−0.0045 (7)	−0.0016 (7)
C6	0.0486 (10)	0.0593 (10)	0.0619 (10)	−0.0010 (8)	−0.0077 (8)	0.0091 (8)
C7	0.0521 (11)	0.0606 (11)	0.0654 (11)	−0.0055 (9)	−0.0025 (9)	0.0130 (9)
C8	0.0451 (9)	0.0436 (9)	0.0440 (8)	0.0034 (7)	−0.0024 (7)	−0.0047 (7)
C9	0.0441 (10)	0.0537 (10)	0.0532 (9)	−0.0038 (8)	−0.0122 (7)	0.0024 (7)
C10	0.0417 (9)	0.0432 (8)	0.0458 (8)	0.0024 (7)	−0.0010 (7)	−0.0068 (7)
C11	0.0419 (9)	0.0387 (8)	0.0488 (8)	0.0033 (7)	−0.0032 (7)	−0.0051 (7)
C12	0.0413 (9)	0.0499 (9)	0.0482 (9)	−0.0032 (7)	0.0000 (7)	−0.0050 (7)
C13	0.0496 (11)	0.0609 (11)	0.0758 (12)	−0.0031 (9)	−0.0059 (9)	0.0032 (9)
C14	0.0452 (11)	0.0817 (14)	0.0811 (13)	−0.0108 (10)	−0.0050 (9)	−0.0029 (11)
C15	0.0602 (13)	0.0795 (14)	0.0732 (12)	−0.0221 (10)	0.0055 (10)	−0.0014 (11)
C16	0.0642 (13)	0.0748 (13)	0.0788 (13)	−0.0189 (10)	−0.0030 (10)	0.0203 (10)
C17	0.0487 (11)	0.0691 (11)	0.0676 (11)	−0.0125 (9)	−0.0078 (8)	0.0128 (9)

Geometric parameters (Å, °)

O1—C2	1.3717 (19)	C5—C8	1.482 (2)
O1—C1	1.416 (2)	C6—C7	1.383 (2)
N1—C10	1.3437 (19)	C6—H6A	0.9300
N1—C11	1.3461 (19)	C7—H7A	0.9300
N2—C8	1.3427 (19)	C8—C9	1.379 (2)
N2—C11	1.3480 (18)	C9—C10	1.388 (2)
N3—C11	1.3433 (19)	C9—H9A	0.9300
N3—H3A	0.8600	C10—C12	1.486 (2)
N3—H3B	0.8600	C12—C13	1.384 (2)
C1—H1B	0.9600	C12—C17	1.384 (2)
C1—H1C	0.9600	C13—C14	1.375 (2)
C1—H1D	0.9600	C13—H13A	0.9300
C2—C7	1.371 (2)	C14—C15	1.376 (3)
C2—C3	1.377 (2)	C14—H14A	0.9300
C3—C4	1.372 (2)	C15—C16	1.368 (3)
C3—H3C	0.9300	C15—H15A	0.9300
C4—C5	1.386 (2)	C16—C17	1.379 (2)
C4—H4A	0.9300	C16—H16A	0.9300
C5—C6	1.380 (2)	C17—H17A	0.9300
C2—O1—C1	118.48 (14)	N2—C8—C9	120.83 (14)
C10—N1—C11	116.15 (13)	N2—C8—C5	116.26 (14)
C8—N2—C11	116.50 (13)	C9—C8—C5	122.92 (14)
C11—N3—H3A	120.0	C8—C9—C10	119.08 (14)
C11—N3—H3B	120.0	C8—C9—H9A	120.5
H3A—N3—H3B	120.0	C10—C9—H9A	120.5
O1—C1—H1B	109.5	N1—C10—C9	120.95 (14)
O1—C1—H1C	109.5	N1—C10—C12	117.16 (13)
H1B—C1—H1C	109.5	C9—C10—C12	121.89 (14)
O1—C1—H1D	109.5	N3—C11—N1	117.58 (13)

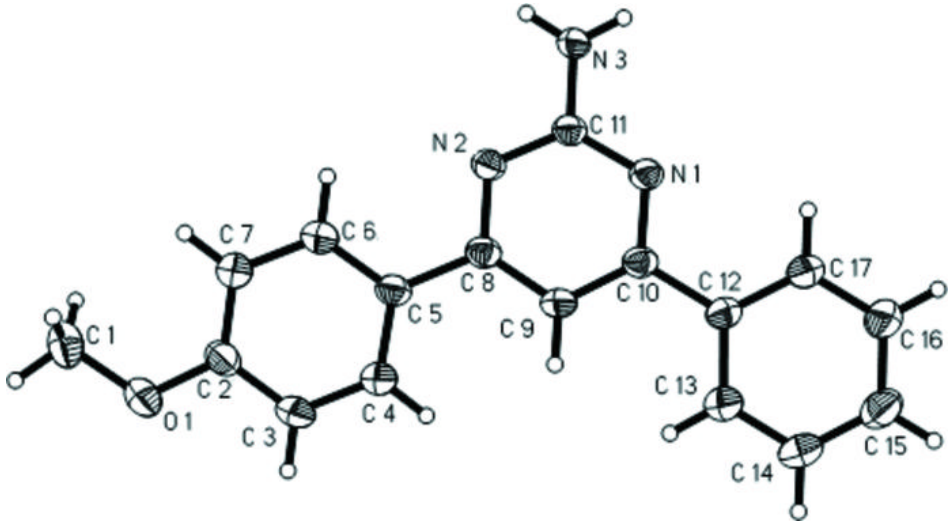
H1B—C1—H1D	109.5	N3—C11—N2	115.96 (13)
H1C—C1—H1D	109.5	N1—C11—N2	126.46 (14)
C7—C2—O1	124.76 (16)	C13—C12—C17	117.17 (15)
C7—C2—C3	119.36 (16)	C13—C12—C10	121.47 (15)
O1—C2—C3	115.87 (15)	C17—C12—C10	121.36 (14)
C4—C3—C2	120.47 (16)	C14—C13—C12	121.53 (17)
C4—C3—H3C	119.8	C14—C13—H13A	119.2
C2—C3—H3C	119.8	C12—C13—H13A	119.2
C3—C4—C5	121.42 (17)	C13—C14—C15	120.42 (18)
C3—C4—H4A	119.3	C13—C14—H14A	119.8
C5—C4—H4A	119.3	C15—C14—H14A	119.8
C6—C5—C4	117.04 (15)	C16—C15—C14	118.94 (18)
C6—C5—C8	120.76 (14)	C16—C15—H15A	120.5
C4—C5—C8	122.20 (15)	C14—C15—H15A	120.5
C5—C6—C7	122.06 (16)	C15—C16—C17	120.58 (19)
C5—C6—H6A	119.0	C15—C16—H16A	119.7
C7—C6—H6A	119.0	C17—C16—H16A	119.7
C2—C7—C6	119.61 (16)	C16—C17—C12	121.35 (17)
C2—C7—H7A	120.2	C16—C17—H17A	119.3
C6—C7—H7A	120.2	C12—C17—H17A	119.3

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···N2^{i}	0.86	2.18	3.012 (3)	163
N3—H3B···N1^{ii}	0.86	2.40	3.191 (3)	154
C6—H6A···N2	0.93	2.47	2.795 (3)	101
C17—H17A···N1	0.93	2.50	2.822 (3)	101

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) −*x*, *y*−1/2, −*z*+1/2.

Fig. 1


N 3
C 11
N 2
N 1
C 7
C 6
C 8
C 10
C 12
C 17
C 5
C 9
C 1
C 16
C 2
C 13
O 1
C 4
C 3
C 15
C 14