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3-Benzyl-6-bromo-2-(2-furyl)-3*H*-imidazo[4,5-*b*]pyridine

Younès Ouzidan,[a] Youssef Kandri Rodi,[a] Hafid Zouihri,[b] El Mokhtar Essassi[c] and Seik Weng Ng[d]*

[a]Laboratoire de Chimie Organique Appliquée, Faculté des Sciences et Techniques, Université Sidi Mohamed Ben Abdallah, Fès, Morocco, [b]CNRST Division UATRS, Angle Allal Fassi/FAR, BP 8027 Hay Riad, Rabat, Morocco, [c]Laboratoire de Chimie Organique Hétérocyclique, Pôle de Compétences Pharmacochimie, Université Mohammed V-Agdal, BP 1014 Avenue Ibn Batout, Rabat, Morocco, and [d]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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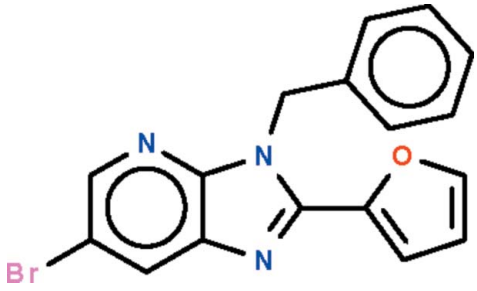
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.031; wR factor = 0.110; data-to-parameter ratio = 13.1.

In the title molecule, $C_{17}H_{12}BrN_3O$, the imidazopyridine ring system is almost coplanar with the furan ring [dihedral angle = 2.0 (3)°]. The benzyl phenyl ring is oriented at dihedral angles of 85.2 (2) and 85.5 (1)°, respectively, with respect to the furan ring and the imidazopyridine ring system. In the crystal, molecules are linked into chains propagating along the *b* axis by C—H···N hydrogen bonds. Adjacent chains are linked *via* short Br···Br contacts [3.493 (1) Å].

Related literature

For a related structure, see: Ouzidan *et al.* (2010).



Experimental

Crystal data

$C_{17}H_{12}BrN_3O$
M_r = 354.21
Monoclinic, $P2_1/c$
a = 15.8422 (3) Å
b = 5.4747 (1) Å
c = 18.4243 (3) Å
β = 111.509 (1)°
V = 1486.68 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.77 mm^{-1}
T = 293 K
0.25 × 0.25 × 0.10 mm

Data collection

Bruker X8 APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.544, T_{max} = 0.769
19471 measured reflections
2614 independent reflections
2105 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.110
S = 0.97
2614 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N3^{i}	0.93	2.51	3.399 (4)	160

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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: CI5113).

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supporting information

Acta Cryst. (2010). E**66**, o1874 [doi:10.1107/S160053681002475X]

3-Benzyl-6-bromo-2-(2-furyl)-3*H*-imidazo[4,5-*b*]pyridine

Younès Ouzidan, Youssef Kandri Rodi, Hafid Zouihri, El Mokhtar Essassi and Seik Weng Ng

S1. Comment

The imidazo[4,5-*b*]pyridine unit is an important heterocyclic nucleus found in a large number of molecules in medicinal chemistry. Heterocycles derived from such compounds posess useful medicinal properties. Owing to their importance, strategies have been developed for their synthesis. The most popular synthetic approach involves the cyclocondensation of 2,3-pyridinediamine with carboxylic acid derivatives or on condensation with aldehydes. An earlier study reported the crystal structure of 4-benzyl-6-bromo-2-phenyl-4*H*-imidazo[4,5-*b*]pyridine (Ouzidan *et al.*, 2010), which was synthesized by using a much more convenient route. The synthesis is extended to the title compound.

In the title molecule (Scheme and Fig. 1), the imidazopyridine ring system is almost coplanar with the furan ring at the 2-position of the five-membered ring [dihedral angle = 2.0 (3) °]. The molecules are linked into chains along the *b* axis by C—H···N hydrogen bonds (Table 1). The adjacent chains are linked via short Br···Br contacts [3.493 (1) Å].

S2. Experimental

6-Bromo-2-furyl-3*H*-imidazo[4,5-*b*]pyridine (0.30 g, 1.13 mmol) was dissolved in DMF (15 ml). Potassium carbonate (0.2 g, 1,48 mmol), tetra-*n*-butylammonium bromide (0.04 g, 0.1 mmol) and benzyl chloride (0.15 ml, 1.36 mmol) were added. Stirring was continued at room temperature for 12 h. The mixture was filtered and the solvent removed under reduced pressure. The residue was chromatographed on a column of silica gel with ethyl acetate-hexane (1/2) as eluent. The compound was recrystallized from chloroform to give orange crystals.

S3. Refinement

H atoms were placed in calculated positions (C–H = 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

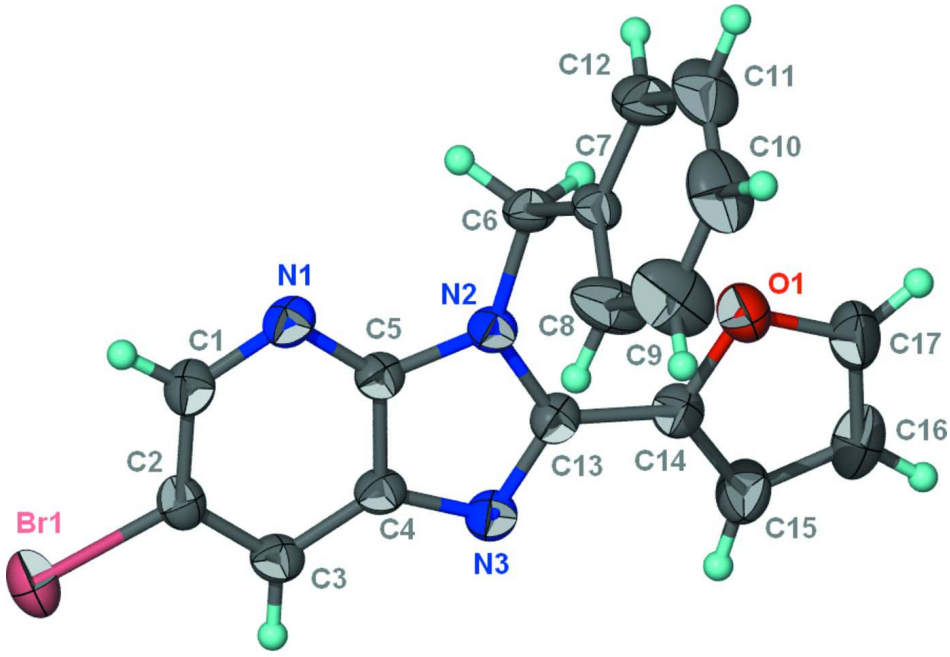

Figure 1

Displacement ellipsoid plot (Barbour, 2001) of the molecule of $C_{17}H_{12}BrN_3O$ at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

3-Benzyl-6-bromo-2-(2-furyl)-3*H*-imidazo[4,5-*b*]pyridine

Crystal data

$C_{17}H_{12}BrN_3O$
$M_r = 354.21$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.8422\ (3)$ Å
$b = 5.4747\ (1)$ Å
$c = 18.4243\ (3)$ Å
$\beta = 111.509\ (1)°$
$V = 1486.68\ (5)$ Å^3
$Z = 4$
$F(000) = 712$
$D_x = 1.583$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5830 reflections
$\theta = 2.7–23.3°$
$\mu = 2.77$ mm^{-1}
$T = 293$ K
Prism, orange
0.25 × 0.25 × 0.10 mm

Data collection

Bruker X8 APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.544$, $T_{max} = 0.769$
19471 measured reflections
2614 independent reflections
2105 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -17\rightarrow18$
$k = -6\rightarrow5$
$l = -21\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.110$
$S = 0.97$
2614 reflections
199 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0848P)^2 + 0.0891P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.47189 (2)	1.27997 (6)	0.426257 (19)	0.05859 (18)
O1	0.21672 (14)	0.1051 (4)	0.11117 (12)	0.0605 (6)
N1	0.28026 (15)	0.7379 (4)	0.34628 (14)	0.0407 (6)
N2	0.26035 (13)	0.4610 (4)	0.23929 (12)	0.0362 (5)
N3	0.37245 (14)	0.6006 (4)	0.20155 (13)	0.0415 (5)
C1	0.33253 (18)	0.9234 (5)	0.38466 (16)	0.0437 (6)
H1	0.3214	0.9916	0.4265	0.052*
C2	0.40263 (16)	1.0193 (5)	0.36533 (15)	0.0399 (6)
C3	0.42374 (17)	0.9297 (5)	0.30393 (15)	0.0400 (6)
H3	0.4701	0.9949	0.2904	0.048*
C4	0.37115 (19)	0.7370 (4)	0.26428 (18)	0.0364 (6)
C5	0.30126 (16)	0.6536 (5)	0.28810 (15)	0.0347 (6)
C6	0.18408 (17)	0.3215 (5)	0.24445 (16)	0.0398 (6)
H6A	0.1851	0.3335	0.2973	0.048*
H6B	0.1923	0.1509	0.2344	0.048*
C7	0.09249 (16)	0.4032 (4)	0.18891 (15)	0.0373 (6)
C8	0.0798 (2)	0.6091 (6)	0.1437 (2)	0.0660 (9)
H8	0.1294	0.7050	0.1467	0.079*
C9	−0.0063 (3)	0.6757 (7)	0.0935 (3)	0.0863 (13)
H9	−0.0139	0.8138	0.0623	0.104*
C10	−0.0799 (2)	0.5399 (7)	0.0897 (2)	0.0752 (10)
H10	−0.1375	0.5839	0.0556	0.090*
C11	−0.0687 (2)	0.3409 (8)	0.1356 (2)	0.0706 (10)
H11	−0.1190	0.2505	0.1340	0.085*
C12	0.0171 (2)	0.2703 (5)	0.1851 (2)	0.0549 (8)
H12	0.0239	0.1319	0.2160	0.066*
C13	0.30648 (16)	0.4385 (5)	0.18846 (15)	0.0369 (6)
C14	0.2871 (2)	0.2623 (4)	0.12615 (18)	0.0428 (7)
C15	0.3289 (2)	0.2287 (6)	0.0754 (2)	0.0587 (9)
H15	0.3787	0.3147	0.0737	0.070*
C16	0.2825 (2)	0.0376 (6)	0.02513 (19)	0.0651 (9)
H16	0.2956	−0.0266	−0.0163	0.078*
C17	0.2169 (3)	−0.0318 (6)	0.04850 (19)	0.0683 (9)
H17	0.1761	−0.1570	0.0257	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0540 (3)	0.0519 (2)	0.0593 (3)	−0.00676 (12)	0.00831 (18)	−0.01181 (13)
O1	0.0659 (14)	0.0602 (13)	0.0594 (14)	−0.0183 (11)	0.0276 (11)	−0.0162 (10)
N1	0.0330 (13)	0.0534 (13)	0.0395 (14)	0.0029 (9)	0.0176 (11)	−0.0003 (10)
N2	0.0268 (11)	0.0449 (11)	0.0378 (13)	−0.0025 (9)	0.0130 (9)	−0.0003 (9)
N3	0.0317 (12)	0.0538 (14)	0.0424 (13)	−0.0020 (10)	0.0175 (10)	−0.0037 (10)
C1	0.0380 (15)	0.0519 (15)	0.0416 (16)	0.0036 (12)	0.0150 (12)	−0.0047 (12)
C2	0.0330 (14)	0.0416 (13)	0.0391 (16)	0.0017 (11)	0.0061 (12)	−0.0006 (11)
C3	0.0296 (14)	0.0464 (14)	0.0440 (16)	−0.0006 (11)	0.0135 (12)	0.0030 (11)
C4	0.0281 (15)	0.0436 (14)	0.0396 (17)	0.0007 (10)	0.0147 (13)	0.0028 (11)
C5	0.0253 (13)	0.0419 (13)	0.0361 (15)	0.0025 (10)	0.0101 (11)	0.0027 (11)
C6	0.0345 (15)	0.0458 (14)	0.0414 (16)	−0.0046 (11)	0.0165 (13)	0.0047 (11)
C7	0.0288 (13)	0.0408 (13)	0.0437 (16)	−0.0052 (10)	0.0152 (12)	−0.0047 (11)
C8	0.0388 (17)	0.063 (2)	0.086 (2)	−0.0040 (14)	0.0108 (17)	0.0219 (17)
C9	0.062 (2)	0.069 (2)	0.102 (3)	0.0088 (19)	−0.001 (2)	0.025 (2)
C10	0.0368 (19)	0.089 (3)	0.083 (3)	0.0077 (17)	0.0013 (17)	−0.012 (2)
C11	0.0350 (19)	0.093 (3)	0.081 (3)	−0.0156 (17)	0.0181 (19)	−0.015 (2)
C12	0.0417 (19)	0.0643 (19)	0.061 (2)	−0.0119 (13)	0.0216 (16)	0.0033 (14)
C13	0.0291 (13)	0.0446 (13)	0.0366 (15)	0.0046 (10)	0.0116 (11)	0.0011 (11)
C14	0.0353 (16)	0.0481 (15)	0.0427 (18)	0.0018 (11)	0.0117 (13)	−0.0002 (11)
C15	0.053 (2)	0.074 (2)	0.054 (2)	−0.0036 (14)	0.0244 (18)	−0.0152 (15)
C16	0.076 (2)	0.070 (2)	0.049 (2)	0.0112 (18)	0.0221 (17)	−0.0105 (15)
C17	0.091 (3)	0.0550 (18)	0.054 (2)	−0.0113 (18)	0.0199 (19)	−0.0155 (15)

Geometric parameters (Å, º)

Br1—C2	1.897 (3)	C7—C8	1.372 (4)
O1—C14	1.355 (3)	C7—C12	1.377 (4)
O1—C17	1.378 (4)	C8—C9	1.387 (5)
N1—C5	1.317 (3)	C8—H8	0.93
N1—C1	1.337 (3)	C9—C10	1.362 (5)
N2—C5	1.383 (3)	C9—H9	0.93
N2—C13	1.388 (3)	C10—C11	1.351 (5)
N2—C6	1.462 (3)	C10—H10	0.93
N3—C13	1.324 (3)	C11—C12	1.385 (5)
N3—C4	1.382 (4)	C11—H11	0.93
C1—C2	1.388 (4)	C12—H12	0.93
C1—H1	0.93	C13—C14	1.444 (4)
C2—C3	1.382 (4)	C14—C15	1.341 (5)
C3—C4	1.376 (4)	C15—C16	1.412 (4)
C3—H3	0.93	C15—H15	0.93
C4—C5	1.408 (4)	C16—C17	1.317 (5)
C6—C7	1.505 (4)	C16—H16	0.93
C6—H6A	0.97	C17—H17	0.93
C6—H6B	0.97		

C14—O1—C17	105.2 (2)	C7—C8—C9	120.7 (3)
C5—N1—C1	113.9 (2)	C7—C8—H8	119.7
C5—N2—C13	105.62 (19)	C9—C8—H8	119.7
C5—N2—C6	123.9 (2)	C10—C9—C8	120.3 (4)
C13—N2—C6	130.5 (2)	C10—C9—H9	119.8
C13—N3—C4	105.2 (2)	C8—C9—H9	119.8
N1—C1—C2	123.4 (3)	C11—C10—C9	119.6 (3)
N1—C1—H1	118.3	C11—C10—H10	120.2
C2—C1—H1	118.3	C9—C10—H10	120.2
C3—C2—C1	122.2 (2)	C10—C11—C12	120.6 (3)
C3—C2—Br1	119.38 (19)	C10—C11—H11	119.7
C1—C2—Br1	118.46 (19)	C12—C11—H11	119.7
C4—C3—C2	115.2 (2)	C7—C12—C11	120.6 (3)
C4—C3—H3	122.4	C7—C12—H12	119.7
C2—C3—H3	122.4	C11—C12—H12	119.7
C3—C4—N3	131.8 (2)	N3—C13—N2	113.1 (2)
C3—C4—C5	118.4 (3)	N3—C13—C14	121.1 (2)
N3—C4—C5	109.9 (2)	N2—C13—C14	125.8 (2)
N1—C5—N2	126.8 (2)	C15—C14—O1	110.5 (3)
N1—C5—C4	127.0 (2)	C15—C14—C13	129.1 (3)
N2—C5—C4	106.2 (2)	O1—C14—C13	120.3 (3)
N2—C6—C7	114.5 (2)	C14—C15—C16	106.7 (3)
N2—C6—H6A	108.6	C14—C15—H15	126.6
C7—C6—H6A	108.6	C16—C15—H15	126.6
N2—C6—H6B	108.6	C17—C16—C15	106.4 (3)
C7—C6—H6B	108.6	C17—C16—H16	126.8
H6A—C6—H6B	107.6	C15—C16—H16	126.8
C8—C7—C12	118.1 (3)	C16—C17—O1	111.2 (3)
C8—C7—C6	123.2 (2)	C16—C17—H17	124.4
C12—C7—C6	118.6 (2)	O1—C17—H17	124.4

C5—N1—C1—C2	0.0 (4)	C6—C7—C8—C9	−180.0 (3)
N1—C1—C2—C3	0.2 (4)	C7—C8—C9—C10	1.4 (7)
N1—C1—C2—Br1	−179.2 (2)	C8—C9—C10—C11	0.7 (7)
C1—C2—C3—C4	−0.8 (4)	C9—C10—C11—C12	−1.7 (6)
Br1—C2—C3—C4	178.56 (19)	C8—C7—C12—C11	1.3 (5)
C2—C3—C4—N3	−179.3 (3)	C6—C7—C12—C11	179.1 (3)
C2—C3—C4—C5	1.2 (4)	C10—C11—C12—C7	0.7 (6)
C13—N3—C4—C3	179.7 (3)	C4—N3—C13—N2	0.5 (3)
C13—N3—C4—C5	−0.7 (3)	C4—N3—C13—C14	179.9 (2)
C1—N1—C5—N2	178.7 (2)	C5—N2—C13—N3	0.0 (3)
C1—N1—C5—C4	0.4 (4)	C6—N2—C13—N3	179.7 (2)
C13—N2—C5—N1	−179.0 (2)	C5—N2—C13—C14	−179.4 (2)
C6—N2—C5—N1	1.3 (4)	C6—N2—C13—C14	0.3 (4)
C13—N2—C5—C4	−0.4 (3)	C17—O1—C14—C15	0.7 (4)
C6—N2—C5—C4	179.9 (2)	C17—O1—C14—C13	179.1 (3)
C3—C4—C5—N1	−1.1 (4)	N3—C13—C14—C15	1.2 (5)
N3—C4—C5—N1	179.3 (2)	N2—C13—C14—C15	−179.5 (3)

C3—C4—C5—N2	−179.7 (2)	N3—C13—C14—O1	−176.9 (2)
N3—C4—C5—N2	0.7 (3)	N2—C13—C14—O1	2.4 (4)
C5—N2—C6—C7	96.8 (3)	O1—C14—C15—C16	−0.3 (4)
C13—N2—C6—C7	−82.8 (3)	C13—C14—C15—C16	−178.5 (3)
N2—C6—C7—C8	−7.5 (4)	C14—C15—C16—C17	−0.3 (4)
N2—C6—C7—C12	174.8 (2)	C15—C16—C17—O1	0.7 (4)
C12—C7—C8—C9	−2.3 (5)	C14—O1—C17—C16	−0.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N3^{i}	0.93	2.51	3.399 (4)	160

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