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2-(3-Bromo-4-methoxyphenyl)imidazo-[1,2-*a*]pyridine

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.051
wR factor = 0.132
Data-to-parameter ratio = 13.3

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

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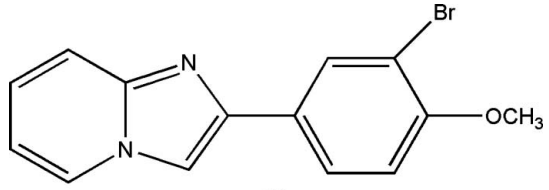
The title compound, $C_{14}H_{11}BrN_2O$, crystallizes with two independent molecules in the asymmetric unit. The dihedral angles between the planes of the imidazo[1,2-*a*]pyridine and benzene rings in the two independent molecules are 2.7 (3) and 12.2 (2)°. There are π–π stacking interactions and intramolecular hydrogen-bond interactions in the crystal structure.

Comment

Imidazo[1,2-*a*]pyridine and its derivatives have clinical applications in the treatment of anxiety disorders; Alpidem (Georges *et al.*, 1993) and Zolpidem (Depoortere *et al.*,1986) are in this category. The title compound, (I), crystallizes with two independent molecules in the asymmetric unit (Fig. 1). All bond lengths and angles in both molecules are within normal ranges (Table 1) and are comparable to those in published structures (Rydzkowski *et al.*, 1988; Zhang & Hu, 2005).



(I)

The dihedral angles between the planes of the imidazo[1,2-*a*]pyridine and benzene rings in the two independent molecules are 2.7 (3) and 12.2 (2)°. The crystal structure contains

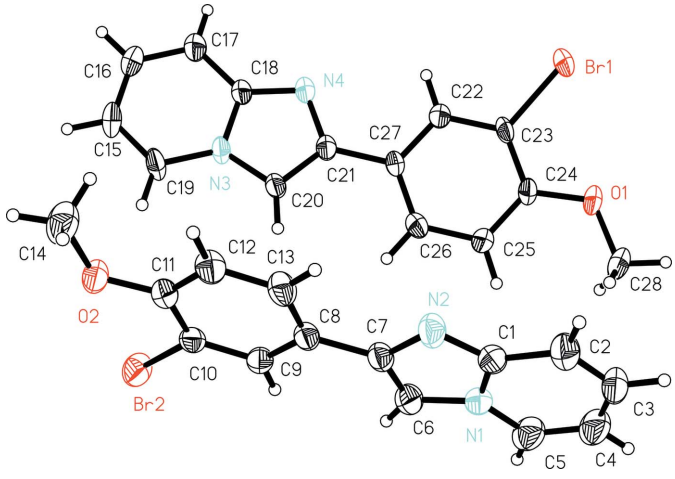


Figure 1
The asymmetric unit of (I), with displacement ellipsoids drawn at the 40% probability level.

π–π stacking interactions and intramolecular C—H···N hydrogen-bond interactions (Table 2). The pyridine ring (C1–C5/N1) stacks with a benzene ring (C8–C13) related by the symmetry operation $(2 - x, -y, -z)$, such that the distance between the ring centroids is 3.681 (5) Å.

Experimental

The title compound was synthesized from 2-bromo-1-(3-bromo-4-methoxyphenyl)ethanone (0.01 mol) and 2-aminopyridine (0.01 mol) in dimethylformamide (20 ml) at 393–403 K for 24 h in a yield of 56% (1.69 g). Crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of a methanol solution at room temperature over a period of two weeks.

Crystal data

$C_{14}H_{11}BrN_2O$
$M_r = 303.16$
Triclinic, $P\overline{1}$
$a = 9.766$ (3) Å
$b = 10.355$ (3) Å
$c = 13.017$ (4) Å
$\alpha = 81.669$ (4)°
$\beta = 74.176$ (4)°
$\gamma = 81.141$ (4)°
$V = 1244.0$ (7) Å^3
$Z = 4$
$D_x = 1.619$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1528 reflections
$\theta = 2.4$–22.4°
$\mu = 3.29$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.45 × 0.34 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.293$, $T_{max} = 0.501$
6527 measured reflections
4317 independent reflections
3163 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.0°$
$h = -11 \rightarrow 11$
$k = -9 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.132$
$S = 0.99$
4317 reflections
325 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.072P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -1.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C23	1.890 (4)	N3—C20	1.362 (5)
Br2—C10	1.891 (4)	N3—C19	1.375 (5)
N4—C18	1.335 (5)	N3—C18	1.388 (5)
N4—C21	1.372 (5)		
C18—N4—C21	105.0 (3)	C1—N2—C7	105.1 (4)

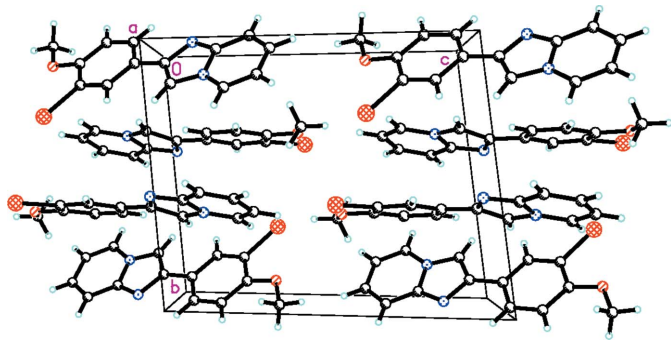


Figure 2
A packing diagram, viewed down the *a* axis.

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13A···N2	0.93	2.56	2.889 (6)	101
C22—H22A···N4	0.93	2.57	2.891 (5)	101

All H atoms were placed in calculated positions, with C—H = 0.93–0.96 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ for the aryl H atoms and $1.5U_{eq}(C)$ for the methyl H atoms. The minimum electron-density peak was located 0.92 Å from atom Br2.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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