Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6-Bromo-3-(2-methylpropenyl)imidazo-[1,2-*a*]pyridine

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.114
Data-to-parameter ratio = 17.5

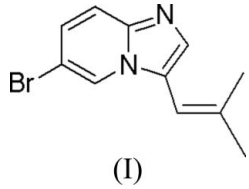
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 22 September 2005
Accepted 31 October 2005
Online 10 November 2005

The title compound, $C_{11}H_{11}BrN_2$, is a new imidazo[1,2-*a*]pyridine-conjugated alkene derivative. It contains a planar imidazo[1,2-*a*]pyridine ring system and a vinyl double bond, which is not in the plane of the heterocycle.

Comment

Imidazo[1,2-*a*]pyridine derivatives are important intermediates in organic synthesis, especially in the synthesis of biologically active and medicinally useful agents. For instance, they are widely used in the synthesis of cyclin-dependent kinase (CDK) inhibitors (Anderson *et al.*, 2003), sleep inducers (Hempel *et al.*, 1996), anticonvulsant agents (Trapani *et al.*, 2003) and antiviral agents (Gueiffier *et al.*, 1996; Gueiffier *et al.*, 1998; Mavel *et al.*, 2002) *etc*. Our group is interested in imidazo[1,2-*a*]pyridine derivatives due to their potential biological profile. We have developed a new method to obtain conjugated alkene derivatives of imidazo[1,2-*a*]pyridine. The title compound, (I), was prepared from the reaction of 6-bromoimidazo[1,2-*a*]pyridine with isobutyraldehyde in the presence of acetic acid.



(I)

The torsion angles of the atoms in the imidazopyridine ring system show that the heterocycle is almost planar. The C10—C11 distance of 1.326 (4) is in the range of a double bond. The N4—C3—C10—C11 torsion angle of −149.6 (3) shows that the vinyl double bond is not in the plane of the heterocycle.

Experimental

6-Bromoimidazo[1,2-*a*]pyridine (0.26 g) was reacted with 7 equivalents of isobutyraldehyde (0.85 ml) in acetic acid (1.5 ml) in a sealed tube at 403 K for 10 h. After cooling to room temperature, the reaction mixture was diluted with water and made basic with saturated sodium carbonate solution. The solution was extracted with dichloromethane, and the organic layer was dried over anhydrous Na_2SO_4. After evaporation of the solvent, the residue was chromatographed using silica gel (petroleum ether: ethyl acetate = 3:1) to afford the pure product, which was dissolved in dichloromethane. Diffraction-quality crystals were obtained by slow evaporation at room temperature.

Crystal data

$C_{11}H_{11}BrN_2$	$Z = 2$
$M_r = 251.13$	$D_x = 1.610$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 6.5532$ (6) Å	Cell parameters from 2749 reflections
$b = 7.594$ (1) Å	$\theta = 2.7$–$27.5°$
$c = 11.026$ (1) Å	$\mu = 3.94$ mm^{-1}
$\alpha = 87.773$ (3)°	$T = 295$ (1) K
$\beta = 73.715$ (2)°	Chunk, colourless
$\gamma = 79.578$ (4)°	0.30 × 0.28 × 0.26 mm
$V = 518.0$ (1) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	2338 independent reflections
ω scans	1906 reflections with $F^2 > 2\sigma(F^2)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.042$
$T_{min} = 0.323$, $T_{max} = 0.359$	$\theta_{max} = 27.5°$
4757 measured reflections	$h = -8 \rightarrow 8$
	$k = -9 \rightarrow 9$
	$l = -14 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[0.0014F_o^2 + 1.3\sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.114$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.42$ e Å^{-3}
2243 reflections	Extinction correction: Larson (1970), equation 22
128 parameters	Extinction coefficient: 27 (7)
H-atom parameters constrained	

The methyl H atoms were positioned with idealized geometry and allowed to rotate but not to tip, with C—H distances of 0.96 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). All other H atoms were placed in geometrically idealized positions with C—H distances of 0.98 Å and were refined using a riding model, with U_{iso}(H) =1.2U_{eq}(C).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP3 for Windows* (Farrugia,1997); software used to prepare material for publication: *CrystalStructure*.

The authors are grateful to the Mr Jianming Gu of the analysis center of Zhejiang University.

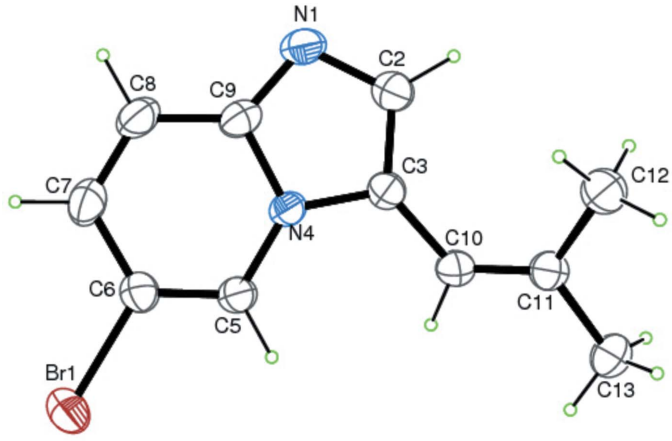


Figure 1
View of the molecule of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level.

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