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5-Bromo-2-iodopyrimidine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
R factor = 0.048
wR factor = 0.091
Data-to-parameter ratio = 14.6

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

The title compound, $C_4H_2BrIN_2$, is a useful intermediate for various sytheses. The complete molecule is located on a crystallographic mirror plane.

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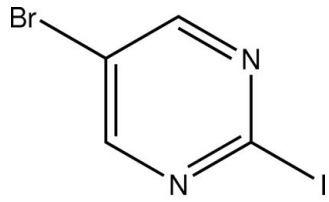
Comment

Pyrimidine is a useful intermediate in selective palladium-catalysed cross-coupling reactions for efficient convergent syntheses. Some derivatives of pyrimidine have superior photoluminescence properties to a conjungated system with alternating triple bonds and aromatic rings (Wong *et al.*, 2001). Some show high efficacy as electron-transporting and photo-polymerizable liquid crystals (Vlachos *et al.*, 2002). Some can be used for blue-light-emitting materials (Wong *et al.*, 2002). The molecular structure of (I) is shown in Fig. 1. The complete molecule is located on a crystallographic mirror plane.



(I)

Experimental

The title compound was synthesized according to the literature method of Goodby *et al.* (1996). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_4H_2BrIN_2$
M_r = 284.88
Orthorhombic, *Pnma*
a = 6.1410 (12) Å
b = 6.7890 (14) Å
c = 16.071 (3) Å
V = 670.0 (2) Å^3
Z = 4
D_x = 2.824 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 10.64 mm^{-1}
T = 293 (2) K
Block, colourless
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.290, T_{max} = 0.345
716 measured reflections
716 independent reflections
392 reflections with $I > 2\sigma(I)$
θ_{max} = 25.9°
3 standard reflections
every 200 reflections
intensity decay: none

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Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.091$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.52$ e Å^{-3}
716 reflections	$\Delta\rho_{min} = -0.51$ e Å^{-3}
49 parameters	

All H atoms were positioned geometrically (C—H = 0.93 Å) and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

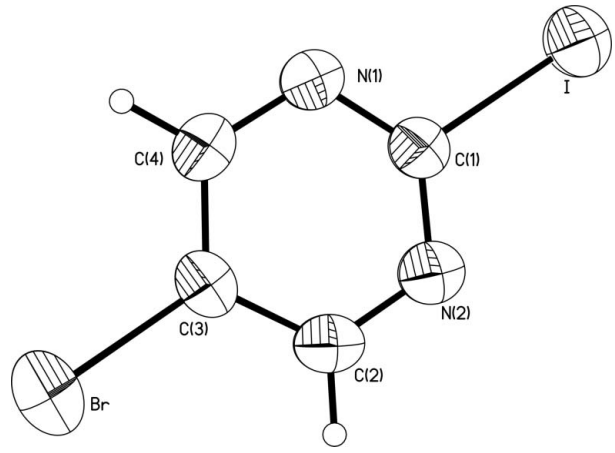

Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

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