

## 3,6-Dibromo-9-isopropyl-9H-carbazole

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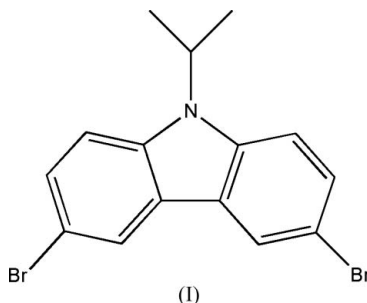
## Key indicators

Single-crystal X-ray study  
 $T = 294\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$   
Disorder in main residue  
 $R$  factor = 0.050  
 $wR$  factor = 0.144  
Data-to-parameter ratio = 16.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $\text{C}_{15}\text{H}_{13}\text{Br}_2\text{N}$ , was synthesized by *N*-alkylation of 2-bromopropane with 3,6-dibromo-9H-carbazole. The carbazole ring system is essentially planar, with a mean deviation of 0.01 Å. The isopropyl group is disordered over two positions across a pseudo-mirror plane perpendicular to the carbazole ring system.

## Comment

Carbazole derivatives substituted by *N*-alkyl groups possess valuable pharmaceutical properties (Buu-Hoï & Royer, 1950; Harfenist & Joyner, 1983; Caulfield *et al.*, 2002; Harper *et al.*, 2002). In this paper, the structure of 3,6-dibromo-9-isopropyl-9H-carbazole, (I), synthesized by *N*-alkylation of 2-bromopropane with 3,6-dibromo-9H-carbazole, is reported.

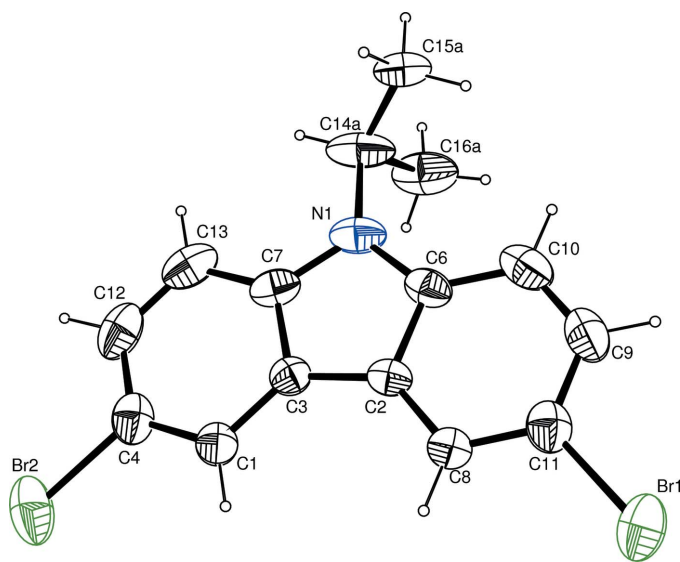


The carbazole ring system of (I) is essentially planar, with a mean deviation of 0.01 Å. The isopropyl group is disordered over two positions across a pseudo-mirror plane perpendicular to the carbazole ring system. The C–Br distances fall in the range 1.898 (7)–1.909 (7) Å, consistent with the literature (Allen *et al.*, 1987; Huang *et al.*, 2005).

## Experimental

The title compound was prepared according to the procedure of Duan *et al.* (2005). A solution of potassium hydroxide (7.0 g) in dimethylformamide (50 ml) was stirred at room temperature for 20 min. 3,6-Dibromocarbazole (6.5 g, 20 mmol), prepared as reported by Smith *et al.* (1992), was added and the mixture stirred for a further 40 min. A solution of 2-bromopropane (3.69 g, 30 mmol) in dimethylformamide (50 ml) was added dropwise with stirring. The resulting mixture was then stirred at room temperature for 12 h and poured into water (500 ml), yielding a white precipitate. The solid product was filtered off, washed with cold water and recrystallized from EtOH, giving crystals of (I) (yield 6.72 g, 91.5%; m.p. 400–401 K). Compound (I) (40 mg) was dissolved in a mixture of chloroform (5 ml) and ethanol (5 ml) and the solution was kept at room temperature for 18 d. Natural evaporation of the solvent gave colourless crystals suitable for X-ray analysis.

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**Figure 1**  
A view of the molecular structure of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. For clarity, only one component of the disordered isopropyl group is shown.

#### Crystal data

$C_{15}H_{13}Br_2N$   
 $M_r = 367.08$   
 Orthorhombic, *Pbca*  
 $a = 16.896$  (2) Å  
 $b = 8.3711$  (10) Å  
 $c = 20.345$  (3) Å  
 $V = 2877.5$  (6) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.695$  Mg m<sup>-3</sup>

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Bruker, 1997)  
 $T_{\min} = 0.398$ ,  $T_{\max} = 0.570$   
 15500 measured reflections

Mo  $K\alpha$  radiation  
 Cell parameters from 3198 reflections  
 $\theta = 2.3$ – $26.0^\circ$   
 $\mu = 5.62$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 Rod, colourless  
 $0.20 \times 0.14 \times 0.10$  mm

3046 independent reflections  
 1605 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.053$   
 $\theta_{\text{max}} = 26.8^\circ$   
 $h = -21 \rightarrow 21$   
 $k = -10 \rightarrow 6$   
 $l = -25 \rightarrow 24$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.050$   
 $wR(F^2) = 0.144$   
 $S = 1.02$   
 3046 reflections  
 188 parameters  
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 3.6671P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.98$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.62$  e Å<sup>-3</sup>

All H atoms were treated as riding on their parent C atoms, with C–H distances of 0.93 (C<sub>aromatic</sub>), 0.96 (C<sub>methyl</sub>) and 0.98 Å (C<sub>methylene</sub>), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}_{\text{aromatic}}, \text{C}_{\text{methylene}})$  or  $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$ . In the final refinement cycle, the disordered isopropyl group was fixed with occupancy factors of 0.59 and 0.41. Geometrical similarity restraints were applied, together with constraints for equality of displacement parameters for C14a and C14b.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

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