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9-(4-Chlorobenzyl)-9*H*-carbazole

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.083
Data-to-parameter ratio = 15.7

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

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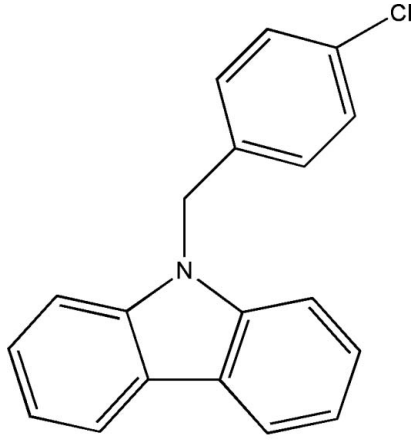
The title compound, $C_{19}H_{14}ClN$, was synthesized by *N*-alkylation of carbazole with 1-chloro-4-(chloromethyl)benzene. The carbazole ring system is essentially planar and makes a dihedral angle of 109.6 (5)° with the plane of the benzene ring.

Comment

Carbazole derivatives substituted by *N*-alkylation 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 9-(4-chlorobenzyl)-9*H*-carbazole, (I) (Fig. 1), is reported. This was synthesized by *N*-alkylation of carbazole with 1-chloro-4-(chloromethyl)-benzene (see *Experimental*).



(I)

The carbazole ring system in (I) is essentially planar, with a mean deviation of 0.0261 Å for non-H atoms. The dihedral angle formed between the carbazole ring system and the plane of the benzene ring (C14–C19) is 109.6 (5)°. The C17—Cl1 distance [1.739 (2) Å] is consistent with the literature, as are all other dimensions (Table 1) (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 298 K for 20 min. Carbazole (3.34 g, 20 mmol) was added and the mixture stirred for a further 40 min. A solution of 1-chloro-4-(chloromethyl)benzene (4.83 g, 30 mmol) in dimethylformamide (50 ml) was added dropwise with stirring. The resulting mixture was then stirred at 298 K 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: 5.26 g (90.2%); 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 298 K. Slow evaporation over a period of 16 d gave colourless crystals suitable for X-ray analysis.

Crystal data

$C_{19}H_{14}ClN$
$M_r = 291.76$
Orthorhombic, $P2_12_12_1$
$a = 5.5571\ (10)$ Å
$b = 13.675\ (3)$ Å
$c = 19.357\ (4)$ Å
$V = 1471.0\ (5)$ Å^3
$Z = 4$
$D_x = 1.317$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2157 reflections
$\theta = 2.6$–$21.2°$
$\mu = 0.25$ mm^{-1}
$T = 294\ (2)$ K
Rod, colourless
0.20 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.951$, $T_{max} = 0.975$
8301 measured reflections
2988 independent reflections
1937 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 26.4°$
$h = -6 \rightarrow 6$
$k = -17 \rightarrow 11$
$l = -21 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.083$
$S = 0.99$
2988 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Absolute structure: Flack (1983), 1233 Friedel pairs
Flack parameter: −0.04 (8)

Table 1
Selected geometric parameters (Å, °).

Cl1—C17	1.739 (2)	C1—C6	1.413 (3)
N1—C1	1.385 (2)	C6—C7	1.438 (3)
N1—C12	1.387 (3)	C7—C12	1.408 (3)
N1—C13	1.463 (3)	C13—C14	1.508 (3)
C1—N1—C12	108.95 (17)	C12—N1—C13	126.00 (18)
C1—N1—C13	125.04 (18)	N1—C13—C14	113.55 (18)

All H atoms were included in the riding model approximation, with C—H distances constrained to 0.93 (aromatic CH) and 0.97 Å (methylene CH_2), and with $U_{iso}(H) = 1.2U_{eq}$(carrier C).

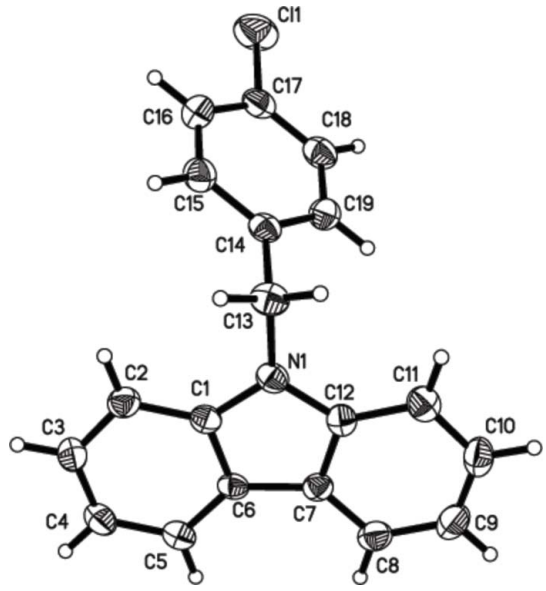


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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