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9-(2,6-Dichlorobenzyl)-9*H*-carbazole

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.096
Data-to-parameter ratio = 13.4

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

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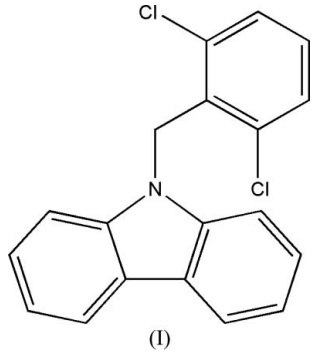
In the title compound, $C_{19}H_{13}Cl_2N$, the dihedral angle between the dichlorobenzyl ring and the carbazole ring system is 92.6 (6)°. In the crystal structure, molecules are linked *via* intermolecular Cl···Cl interactions.

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). This paper reports the structure of the title compound, (I) (Fig. 1), which was synthesized by the *N*-alkylation of carbazole with 1,3-dichloro-2-(chloromethyl)benzene.



(I)

In the molecule of (I), the carbazole ring system is essentially planar, with an r.m.s. deviation from the mean plane of 0.009 Å. The angle between the dichlorobenzyl ring (C1–C6) and the carbazole plane is 92.6 (6)°.

In the crystal structure of (I), dimers are formed through weak intermolecular Cl···Cl^{i} interactions [symmetry code: (i) $-x, 1-y, -z$], with Cl···Cl = 3.449 (5) Å and C5—Cl2···Cl2 angles = 161.9 (5)°. These values are typical for inversion-related Cl···Cl interactions (Desiraju, 1989).

Experimental

Compound (I) was synthesized according to the procedure of Huang *et al.* (2005). Crystals suitable for X-ray analysis were grown by slow evaporation of a solution in a mixture of chloroform (6 ml) and ethanol (2 ml) at room temperature over a period of 11 d.

Crystal data

$C_{19}H_{13}Cl_2N$
M_r = 326.20
Monoclinic, *C*2/*c*
a = 27.291 (6) Å
b = 5.5688 (13) Å
c = 21.132 (5) Å
β = 109.879 (4)°
V = 3020.3 (12) Å^3
Z = 8
D_x = 1.435 Mg m^{-3}
Mo *Kα* radiation
μ = 0.42 mm^{-1}
T = 294 (2) K
Plate, colourless
0.20 × 0.16 × 0.08 mm

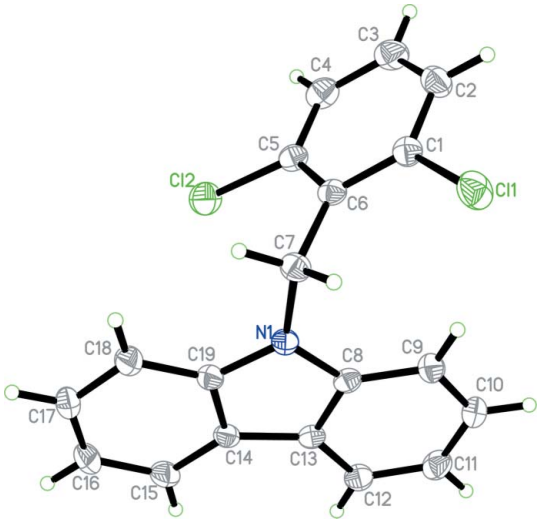


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

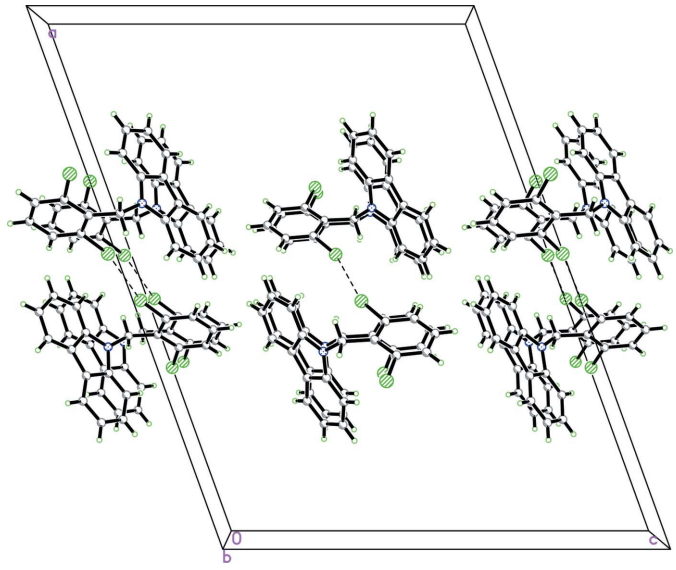


Figure 2
Part of the crystal structure of (I), with Cl···Cl interactions drawn as dashed lines.

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.920, T_{max} = 0.967
7298 measured reflections
2666 independent reflections
1839 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.096
S = 1.01
2666 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.047P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

All H atoms were included in the riding-model approximation, with C—H = 0.93 (aromatic) and 0.97 Å (CH_2), and with U_{iso}(H) = 1.2U_{eq}(C).

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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