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

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.045
wR factor = 0.129
Data-to-parameter ratio = 7.6

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

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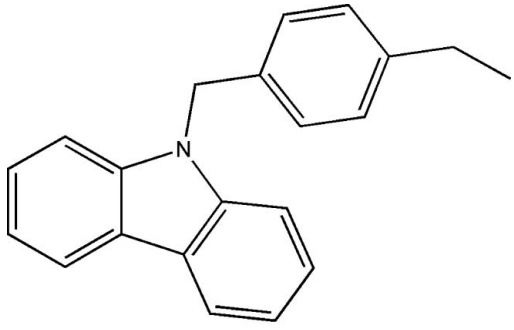
In the title compound, $C_{21}H_{19}N$, the carbazole ring system is essentially planar. The structure is stabilized by both π–π and C—H$\cdots\pi$ interactions. The ethylbenzene ring was found to be disordered.

Comment

Carbazole derivatives possess valuable therapeutic properties. In some cases they are able to potentiate the analgesic effect of, for example, morphine, without substantially influencing the blood pressure and the vegetative nervous system (Chemische Fabrik Promonla GmbH, 1959). *N*-alkylation is an important process for the construction of carbazole derivatives (Duan *et al.*, 2004). The structure of the title compound, $C_{21}H_{19}N$, 9-(4-ethylbenzyl)-9*H*-carbazole, (I), is reported here; it was synthesized by *N*-alkylation of carbazole with 1-(chloromethyl)-4-ethylbenzene.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The carbazole ring system is essentially planar, with a mean deviation of 0.003 Å. The dihedral angle between the carbazole plane and that of the major component of the disordered ethylbenzene ring is 72.3 (5)°. Bond lengths and angles are in agreement with reported literature values (Allen *et al.*, 1987). In the crystal structure, there are weak π–π stacking interactions between the ethylbenzene rings at $(x-\frac{1}{2}, -y+\frac{1}{2}, -z)$ and $(x+\frac{1}{2}, -y+\frac{1}{2}, -z)$; the distance between ring centroids is 5.271 (8) Å. Additional strong C—H$\cdots\pi$ interactions are observed, the distance between H10*a* and the centroid of the C1/C2/C3/C4/C5/C6 plane at $(1-x, -\frac{1}{2}+y, \frac{1}{2}-z)$ being 2.98 Å and that between H13*b* and the centroid of the C7/C8/C9/C10/C11/C12 plane at $(1+x, y, z)$ plane being 2.84 Å.

Experimental

A solution of potassium hydroxide (7.0 g) in DMF (50 ml) was stirred at room temperature for 20 min. Carbazole (3.3 g, 20 mmol) was added and the mixture was stirred for a further 40 min. A solution of

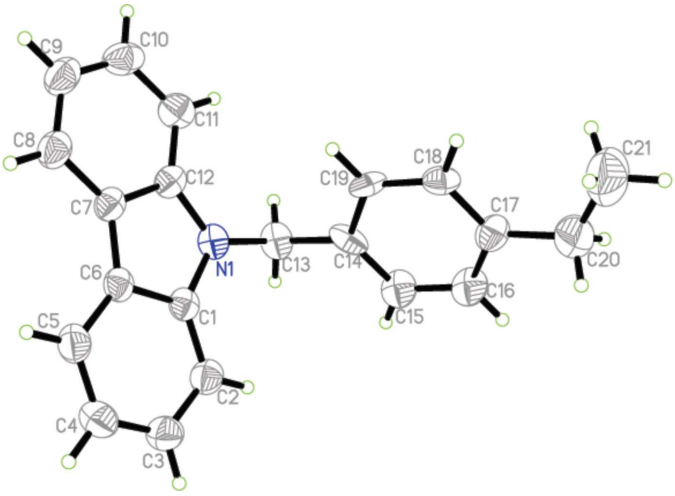


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Only the major component of the disordered ethylbenzene group is shown.

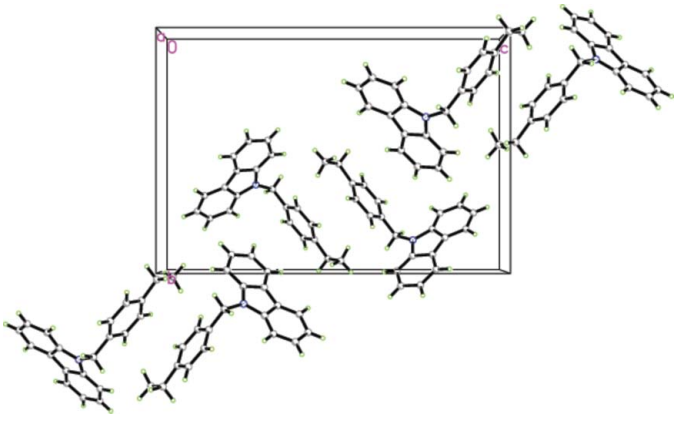


Figure 2
A partial packing diagram for (I). Only the major component of the disordered ethylbenzene group is shown.

1-(chloromethyl)-4-ethylbenzene (8.5 g, 30 mmol) in DMF (50 ml) was added dropwise with stirring. The resulting mixture was stirred at room temperature for 12 h and poured into 500 ml water to give a white solid product. This was filtered, washed with water and recrystallized from EtOH to give (I). Yield: 4.90 g (85.9%); m.p.: 392.5–393.8 K; 20 mg of (I) was dissolved in 6 ml chloroform, and the solution was kept at room temperature for 10 d. Natural evaporation gave colorless single crystals of (I), suitable for X-ray analysis.

Crystal data

$C_{21}H_{19}N$
M_r = 285.37
Orthorhombic, $P2_12_12_1$
a = 5.6074 (14) Å
b = 13.943 (3) Å
c = 20.124 (5) Å
V = 1573.4 (7) Å^3
Z = 4
D_x = 1.205 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1424 reflections
θ = 2.5–20.7°
μ = 0.07 mm^{-1}
T = 294 (2) K
Block, colorless
0.22 × 0.16 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.977, T_{max} = 0.990
8829 measured reflections
1883 independent reflections
1028 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 26.5°
$h = -6 \rightarrow 6$
$k = -17 \rightarrow 10$
$l = -25 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.129
S = 1.00
1883 reflections
249 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.020 (4)

H atoms were included in calculated positions and treated as riding atoms [C—H distances are 0.93 Å for CH and 0.97 Å for CH_2 groups, with U_{iso}(H) = 1.2 U_{eq}(C), and C—H =0.96 Å for methyl groups, with U_{iso}(H) = 1.5 U_{eq}(C). In the absence of significant anomalous dispersion effects, Freidel pairs were merged. The ethylbenzene ring was found to be disordered and refined as a regular hexagon with the C—C distances of 1.39 Å. Site occupancies of the two disorder components, which included the atoms of the benzene ring and its ethyl substituent, refined to 0.521 (12) and 0.479 (12).

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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