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1-{4-[(9-Ethylcarbazolyl)vinyl]phenyl}-1*H*-imidazole

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The molecule of the title compound, $C_{25}H_{21}N_3$, contains three aromatic components and displays a non-planar structure. The dihedral angles between the imidazole and benzene planes and between the benzene and carbazole planes are 19.9 (2) and 24.8 (1)°, respectively.

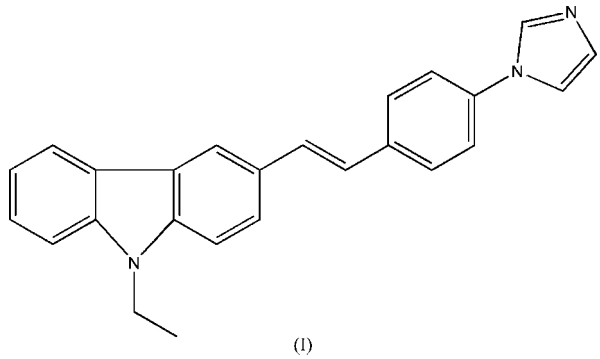
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.056
wR factor = 0.074
Data-to-parameter ratio = 12.8

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

Comment

As part of our ongoing investigation on imidazole derivatives, the title compound, (I), has been prepared and its crystal structure is presented here.



(I)

The molecular structure of (I) is shown in Fig. 1. The molecule of (I) is non-planar; the dihedral angles between the imidazole and benzene planes and between the benzene and carbazole planes are 19.9 (2) and 24.8 (1)°, respectively. The ethyl group is nearly perpendicular to the carbazole plane, the dihedral angle being 68.0 (2)°.

Experimental

For the praparation of the title compound, [(9-ethylcarbazolyl)-methylene]thipheny1phosphonium iodide (5.97 g, 10 mmol), 4-(imidazol-1-yl)benzaldehyde (1.72 g, 10 mmol) and NaOH (2.00 g, 50 mmol) were ground in a mortar for 20 min. The yellow product was purified by column chromatography on silica ge1, using ethy1 acetate/petroleum ether (4:1) as eluent (yie1d: 2.9 g, 80%). Single crystals of (I) were obtained by slow evaporation of a benzene solution at room temperature.

Crystal data

$C_{25}H_{21}N_3$
M_r = 363.45
Monoclinic, $P2_1/c$
a = 9.2975 (19) Å
b = 8.6481 (17) Å
c = 25.394 (7) Å
β = 110.47 (3)°
V = 1912.9 (8) Å^3
Z = 4
D_x = 1.262 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, pale yellow
0.35 × 0.30 × 0.28 mm

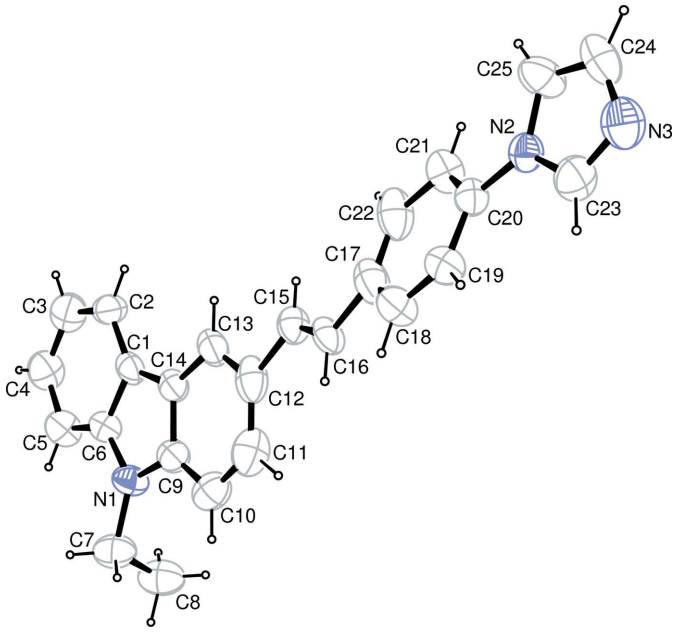


Figure 1
The molecular structure of (I), with 40% probability displacement ellipsoids (arbitrary spheres for H atoms). The minor disorder component has been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

N1—C6	1.404 (4)	N2—C23	1.353 (4)
N1—C7	1.482 (3)	N2—C25	1.343 (4)
N1—C9	1.407 (4)	N3—C23	1.322 (4)
N2—C20	1.439 (4)	N3—C24	1.327 (4)
C6—N1—C9	109.0 (3)	C25—N2—C20	129.6 (4)
C6—N1—C7	125.3 (3)	C23—N2—C20	126.3 (4)
C9—N1—C7	125.6 (4)	C23—N3—C24	103.5 (4)
C25—N2—C23	104.1 (3)		

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and the torsion angle was refined to fit the electron density, U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions, with C—H = 0.97 (methylene) or 0.93 Å (aromatic), and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C). The vinyl group (C15, C16 and attached H atoms) is disordered over two sites; occupancies were refined and converged to 0.588 (10) and 0.412 (10).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
7618 measured reflections
3363 independent reflections
1067 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.074
S = 0.91
3363 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0006P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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