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2-[(1*Z*)-(9-Ethyl-9*H*-carbazol-3-yl)-methyleneamino]-4,5,6,7-tetrahydro-1-benzothiophene-3-carbonitrile–benzene (2/1)

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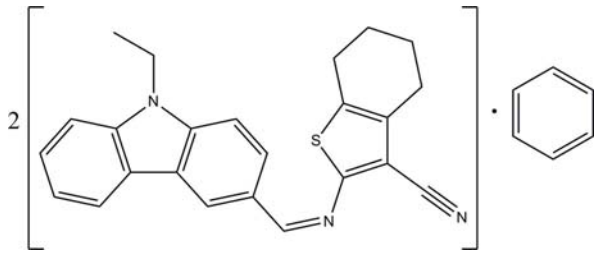
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.070; wR factor = 0.167; data-to-parameter ratio = 22.7.

In the title compound, $2C_{24}H_{21}N_3S\cdot C_6H_6$, the two independent Schiff base molecules (*A* and *B*) in the asymmetric unit differ in the orientation of the tetrahydrobenzothiophene ring system with respect to the carbazole ring system by 180° rotation about the C—C bond in the C—C═N—C linkage. The two molecules also differ in the orientation of the ethyl groups [C—N—C—C torsion angle of 90.7 (3)° in molecule *A*, and −79.4 (3)° in molecule *B*]. In molecule *B*, two methylene C atoms of the cyclohexene ring are disordered over two sites with occupancies of 0.58 (1) and 0.42 (1). The cyclohexene rings in both molecules adopt half-chair conformations. The dihedral angle between the thiophene ring and the carbazole ring system is 8.07 (9)° in molecule *A* [3.10 (9)° in molecule *B*]. In the crystal structure, the independent molecules are linked into dimers by intermolecular C—H···N hydrogen bonds. In addition, C—H···π interactions are observed.

Related literature

For biological and other applications of Schiff base compounds, see: Abu-Hussen (2006); Elerman *et al.* (2002); Panneerselvam *et al.* (2005); Walsh *et al.* (1996). For ring puckering parameters, see: Cremer & Pople (1975). For a related structure, see: Elerman & Elmali (1998).



Experimental

Crystal data

$2C_{24}H_{21}N_3S\cdot C_6H_6$
M_r = 845.10
Triclinic, $P\overline{1}$
a = 11.4816 (1) Å
b = 13.7322 (2) Å
c = 14.8358 (2) Å
α = 81.841 (1)°
β = 77.083 (1)°
γ = 83.864 (1)°
V = 2250.00 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 293 K
0.45 × 0.15 × 0.07 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.931, T_{max} = 0.989
48693 measured reflections
13169 independent reflections
6227 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.167
S = 1.01
13169 reflections
580 parameters
63 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1*B*–C6*B*, C7*A*–C12*A* and C14*A*–C16*A*/C21*A*/S1*A* rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C22*A*—H22*A*···N3*B*^{i}	0.97	2.59	3.487 (3)	155
C11*A*—H11*A*···*Cg*1^{ii}	0.93	2.65	3.499 (3)	153
C11*B*—H11*B*···*Cg*2^{i}	0.93	2.82	3.725 (3)	166
C27—H27*A*···*Cg*3^{iii}	0.93	2.71	3.625 (6)	169

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x-1, y, z$; (iii) $-x, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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