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


Abstract: In the title compound, 2C24H21N3S·C6H6, 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 . . . n interactions are observed.