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(*E*)-3-(9-Ethyl-9*H*-carbazol-3-yl)-1-(2-hydroxyphenyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.145
Data-to-parameter ratio = 14.8

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

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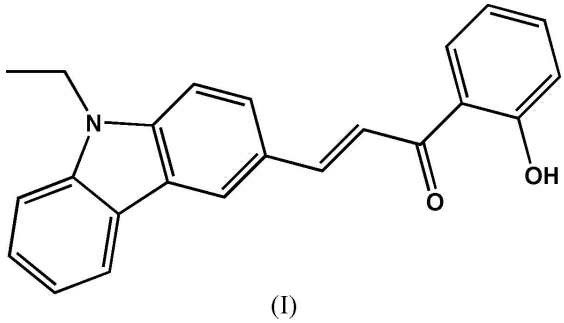
In the crystal structure of the title compound, $C_{23}H_{19}NO_2$, the molecular backbone is nearly planar, with a dihedral angle of 11.58 (12)° between the planes of the carbazole and benzene groups.

Comment

In recent years, considerable interest has been devoted to the synthesis and study of substituted chalcones because of their roles as fluorescent probes (Jiang *et al.*, 1994) and as precursors in the biological formation of flavonoids (Nel *et al.*, 1998), and their potential nonlinear optical properties (Wang & Wu, 1994). In particular, the chalcone derivatives with typical *D*—π—*A* mode have been reported to exhibit intense fluorescence properties. For example, 4′′-dimethylaminochalcone (DMAC) has been reported to be a potential chemosensor (DiCesare & Lakowicz, 2000) when it is substituted by different groups, since its fluorescent properties can be altered by different surrounding conditions. In our previous work, the structure of 2′-hydroxy-DMAC has been reported (Liu *et al.*, 2002). To further understand the structure–property relationship, we synthesized a new DMAC analog with *N*-ethylcarbazolyl as electron-donor group. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I), along with the atom-numbering scheme, is shown in Fig. 1. The molecular backbone is nearly planar, as indicated by the dihedral angle of 11.58 (12)° between the planes of the carbazole and benzene groups. The central propenone group, C15–C17/O1, is planar and coplanar with the carbazole group [dihedral angle 2.94 (9)°], suggesting some π conjugation between the groups. The hydroxybenzoyl moiety is also nearly planar [maximum displacement from the least-squares plane is 0.052 (3) Å for C17], as a result of the presence of some π conjugation and an intramolecular O2—H···O1 hydrogen-bond interaction.

In the crystal structure, the molecules are assembled into a herringbone pattern (Fig. 2). The packing can be described as

consisting of alternate layers perpendicular to the *c* axis, in which the molecules are parallel and arranged in a head-to-tail manner, with a separation of about 3.38 Å, indicating the presence of some π stacking interaction. The molecules of adjacent layers are nearly perpendicular and arranged in a head-to-head manner.

Experimental

A mixture of 2′-hydroxyacetophenone (1.36 g, 0.01 mol) and NaOH (0.48 g, 0.012 mol) was dissolved in ethanol, and then *N*-ethylcarbazole-3-aldehyde (2.2 g, 0.01 mol) in ethanol was added dropwise with stirring. The mixture was heated to reflux for 2 h until a substantial precipitate formed. The precipitate was filtered off and washed twice with ethanol to give the final product. Orange crystals of the title compound, which were suitable for X-ray analysis, were obtained by recrystallization from acetonitrile.

Crystal data

$C_{23}H_{19}NO_2$
M_r = 341.39
Monoclinic, $P2_1/c$
a = 8.9637 (9) Å
b = 24.689 (3) Å
c = 9.0990 (9) Å
β = 117.788 (6)°
V = 1781.5 (3) Å^3
Z = 4
D_x = 1.273 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 41 reflections
θ = 5.1–12.5°
μ = 0.08 mm^{-1}
T = 293 (2) K
Prism, orange
0.58 × 0.34 × 0.20 mm

Data collection

Bruker *P*4 diffractometer
ω scans
Absorption correction: ψ scans (*XSCANS*; Bruker, 1996)
T_{min} = 0.872, T_{max} = 0.983
4385 measured reflections
3491 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°
$h = -11 \rightarrow 1$
$k = -1 \rightarrow 30$
$l = -10 \rightarrow 11$
3 standard reflections every 97 reflections
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.145
S = 0.95
3491 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.026 (2)

Table 1
Selected geometric parameters (Å, °).

C5—C6	1.408 (3)	C13—C15	1.454 (3)
C5—C10	1.441 (3)	C15—C16	1.328 (3)
C6—N1	1.388 (3)	C16—C17	1.457 (3)
C8—N1	1.467 (3)	C17—O1	1.250 (3)
C9—N1	1.378 (3)	C17—C18	1.471 (3)
C9—C10	1.412 (3)	C20—O2	1.347 (3)
C6—C5—C10	106.38 (19)	O1—C17—C16	119.8 (2)
N1—C6—C5	109.15 (19)	O1—C17—C18	119.5 (2)
N1—C9—C10	109.05 (19)	C16—C17—C18	120.6 (2)
C9—C10—C5	106.82 (19)	C9—N1—C6	108.59 (18)
C16—C15—C13	127.7 (2)	C9—N1—C8	125.8 (2)
C15—C16—C17	122.9 (2)	C6—N1—C8	125.5 (2)

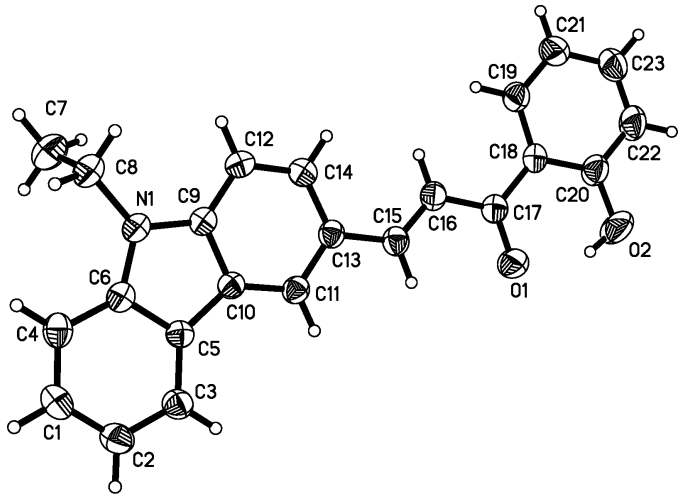


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

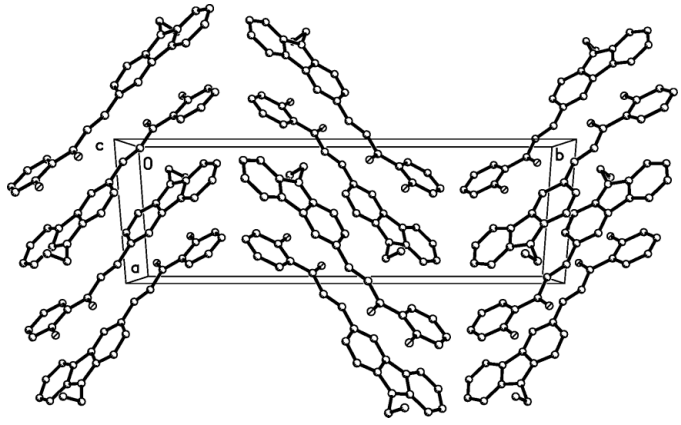


Figure 2
Packing diagram for the title compound, viewed along the *c* axis. H atoms have been omitted.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*B*···O1	0.82	1.78	2.511 (3)	148

After their successful location in a difference map, all H atoms were positioned geometrically and allowed to ride on their attached atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for aryl, CH and CH_2 H atoms, and 1.5U_{eq}(C,O) for OH and CH_3 H atoms.

Data collection: *XSCANS* (Bruker,1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; 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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