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Shu-Jiang Tu,* Yan Zhang and Run-Hong Jia

Department of Chemistry, Xuzhou Normal University, Xuzhou 221116, People's Republic of China

Correspondence e-mail: laotu2001@263.net

Key indicators

Single-crystal X-ray study T = 298 KMean $\sigma(\text{C}-\text{C}) = 0.004 \text{ Å}$ R factor = 0.051 wR factor = 0.140 Data-to-parameter ratio = 11.8

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

13-(4-Fluorophenyl)-12*H*-benzo[*f*]indeno-[1,2-*b*]quinolin-12-one

The title compound, $C_{26}H_{14}FNO$, was synthesized by the reaction of 4-fluorobenzaldehyde, 2-naphthylamine and 1,3indanedione in glycol under microwave irradiation. The pendent fluorophenyl ring makes a dihedral angle of 90.84 (1)° with the adjacent pyridine component of the fused ring system.

Comment

Indenoquinoline derivatives show a wide range of biological properties, such as 5-HT-receptor binding activity, antiinflammatory activity (Lu *et al.*, 2003), and also act as antitumor agents, inhibitors for steroid reductase (Deady *et al.*, 2000), acetylcholinesterase inhibitors, and antimalarials (Rampa *et al.*, 2000). We report here the crystal structure of the title compound, (I), prepared by the reaction of 4fluorobenzaldehyde, 2-naphthylamine and 1,3-indanedione in glycol under microwave irradiation.



The pyridine ring, naphthalene ring and indenone ring all adopt planar conformations (Fig. 1). The dihedral angle between the C1/C9/C10/C11//C20/N1 and C21–C26 planes is 90.84 (1)°. The naphthalene and indenone rings form dihedral angles of 1.3 (2) and 1.1 (2)°, respectively, with the C1/C9/C10/C11//C20/N1 plane.

Experimental

Compound (I) was prepared by the reaction of 4-fluorobenzaldehyde (1 mmol), 2-naphthylamine (1 mmol) and 1,3-indanedione (1 mmol) in glycol (2 ml) under microwave irradiation for 4 min. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 95%; m.p. 573 K).

Crystal data	
C ₂₆ H ₁₄ FNO	$V = 892.8 (4) \text{ Å}^3$
$M_r = 375.38$	Z = 2
Triclinic, $P\overline{1}$	$D_x = 1.396 \text{ Mg m}^{-3}$
a = 7.908 (2) Å	Mo $K\alpha$ radiation
b = 9.935 (3) Å	$\mu = 0.09 \text{ mm}^{-1}$
c = 12.188 (3) Å	T = 298 (2) K
$\alpha = 79.132 \ (4)^{\circ}$	Block, yellow
$\beta = 86.569 \ (5)^{\circ}$	$0.23 \times 0.12 \times 0.09 \text{ mm}$
$\gamma = 71.716 \ (4)^{\circ}$	

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Bruker SMART CCD area-detector diffractometer φ and ω scans Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\min} = 0.979, T_{\max} = 0.992$

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.051$ $wR(F^2) = 0.140$ S = 1.043102 reflections 262 parameters H-atom parameters constrained 4684 measured reflections 3102 independent reflections 1615 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.022$ $\theta_{\text{max}} = 25.0^{\circ}$

$$\begin{split} &w = 1/[\sigma^2(F_{\rm o}^{-2}) + (0.0557P)^2 \\ &+ 0.0462P] \\ &where \ P = (F_{\rm o}^{-2} + 2F_{\rm c}^{-2})/3 \\ (\Delta/\sigma)_{\rm max} < 0.001 \\ \Delta\rho_{\rm max} = 0.25 \ {\rm e} \ {\rm \AA}^{-3} \\ \Delta\rho_{\rm min} = -0.19 \ {\rm e} \ {\rm \AA}^{-3} \end{split}$$



F1

Figure 1



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C-H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve

H atoms were positioned geometrically and treated as riding, with

structure: *SHELXS97* (Sheldrick, 1997); program(s) used to solve structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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