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7-Diethylamino-3-[(2Z)-3-(6-methoxy-2-naphthyl)prop-2-enoyl]-2H-chromen-2-one

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7-Diethylamino-3-[(2*Z*)-3-(6-methoxy-2-naphthyl)prop-2-enoyl]-2*H*-chromen-2-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.151
Data-to-parameter ratio = 14.3

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

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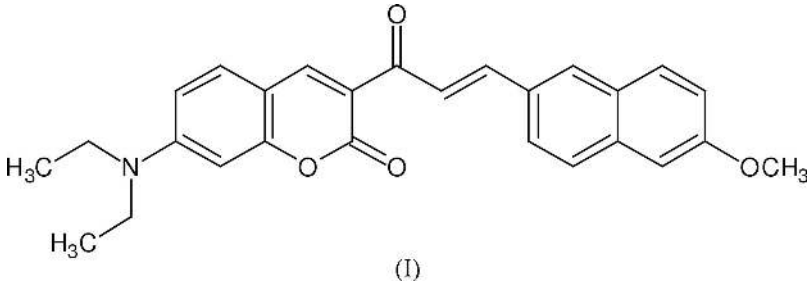
The geometric parameters of the title molecule, $C_{27}H_{25}NO_4$, are in the usual ranges. The central C=C double bond is *trans* configured, with the two C atoms slightly twisted out of the plane of the naphthyl group. The dihedral angle between the two fused ring systems is 40.90 (4)°.

Comment

Compounds incorporating benzopyrone structural units possess a wide range of biological activities (Pawar & Mulwad, 2004). Coumarins are an important class of molecules because of their applications in synthetic chemistry, medicinal chemistry and photochemistry (Vishnumurthy *et al.*, 1996, 1997, 1999). The coumarin system is the basis of various compounds possessing anticoagulant and anti-inflammatory activities (Lin *et al.*, 2006). The crystal structures of some of these types of compoumds have recently been reported in the literature, *viz.* 3-acetyl-7-(diethylamino)coumarin (Hamaker & McCully, 2006), 3-acetyl-6-chloro-2*H*-chromen-2-one (Chopra *et al.*, 2006) and 7-diethylamino-2-oxo-2*H*-chromene-3-carboxylic acid (Bardajee *et al.*, 2006). As part of out current reasearch, we have synthesized and determined the crystal structures of some chalcones (Yathirajan, Sarojini *et al.*, 2006; Yathirajan, Narayana *et al.*, 2006; Yathirajan, Vijaya Raj *et al.*, 2006; Yathirajan, Ashalatha *et al.*, 2006; Yathirajan, Sreevidya *et al.*, 2006; Yathirajan *et al.*, 2007). In a continuation of our quest to synthesize new materials which may find uses in the photonics industry, we report here the crystal structure of a new chalcone, (I), containing a benzopyrone unit.



(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Allen *et al.*, 1987). The carbonyl group is twisted by −9.8 (3)° from the plane of the coumarin unit. The torsion angle between the carbonyl group and the C atoms of the double bond is −14.1 (3)°. The torsion angle between the the C atoms of the double bond and the adjacent naphthyl group (C2—C3—C31—C40) is −7.1 (4)°. The two fused ring systems form a dihedral angle of 40.90 (4)°.

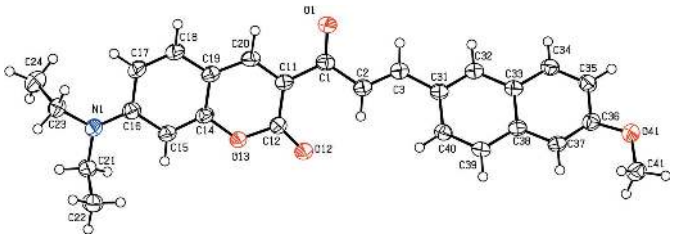


Figure 1
The molecular structure of (I) with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

Experimental

Piperidine (0.5 ml) was added to a thoroughly stirred solution of 7-*N*,*N*-diethylamino-3-acetylcoumarin (2.59 g, 0.01 mol) and 6-methoxy-2-naphthaldehyde (1.86 g, 0.01 mol) in 25 ml ethanol and the mixture was refluxed for 8 h and cooled. The solid which precipitated was filtered off and recrystallized from an acetone–toluene (1:1) mixture (m.p. 479–481 K). Analysis for $C_{27}H_{25}NO_4$ found (calculated): C 75.78 (75.86), H 5.80 (5.89), N 3.20% (3.28%).

Crystal data

$C_{27}H_{25}NO_4$
M_r = 427.48
Monoclinic, $P2_1/c$
a = 20.8426 (13) Å
b = 7.9413 (8) Å
c = 13.5838 (9) Å
β = 107.246 (5)°
V = 2147.3 (3) Å^3
Z = 4
D_x = 1.322 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
Thick plate, red
0.23 × 0.17 × 0.09 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: none
12741 measured reflections
4162 independent reflections
3162 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.151
S = 1.09
4162 reflections
292 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.8794P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

H atoms were found in a difference map, but they were subsequently refined using a riding model, with C—H = 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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