3-(6-Methoxy-2-naphthyl)-1-(2-naphthyl)prop-2-en-1-one

The title compound, C_{24}H_{18}O_{2}, is a chalcone derivative. The torsion angle between the mean planes of the two naphthalene groups is 54.41 (2)^\circ.

Comment

Substituted chalcones have many applications in medicine and physics. (see e.g. Xu et al., 2005). The crystal structures of 1-(2-naphthyl)-3-(4-nitrophenyl)prop-2-en-1-one (Raj et al., 1996) and 3-(4-methylphenyl)-1-(2-naphthyl)prop-2-en-1-one (Moorthi et al., 2005) have been reported. In continuation of our work on chalcones (Yathirajan et al., 2006a,b) the present work reports the crystal structure of the title compound, (I). (Fig. 1).

The bond lengths and angles in (I) can be regarded as normal (Cambridge Crystallographic Database, Version 5.27, November 2005 updated August 2006; MOGUL, Version 1.1; Allen, 2002). The atoms of the C12/C13 double bond and the C14/O2 carbonyl group are almost coplanar with the C1–C10 naphthalene ring system (r.m.s. deviation from the mean plane = 0.173 Å), but the C21–C30 naphthalene ring system is twisted substantially with respect to C12–C14/O2: the dihedral angle between the two naphthalene system ring planes is 54.41 (2)^\circ. There are no π–π stacking interactions in (I).

Experimental

Compound (I) was synthesized according to the method reported in the literature (Vogel, 1989) in a yield of 85%. The compound was

Figure 1

View of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).
purified by recrystallization from ethanol and crystals of (I) were
grown by slow evaporation of an acetone–toluene (50:50 v/v) solution
(m.p. 448–450 K). Analysis found (calc.) (%) for C_{24}H_{18}O_{2}: C: 85.20
(85.18); H: 5.30 (5.36).

Crystal data
C_{24}H_{18}O_{2}
Mr = 338.38
Monoclinic, \( P2_1/n \)
a = 7.5270 (8) \( \AA \)
b = 5.9364 (4) \( \AA \)
c = 37.576 (4) \( \AA \)
\( \beta = 92.046 (8) \) \( ^\circ \)
\( V = 1677.9 (3) \) \( \AA^3 \)

Z = 4
\( D_\lambda = 1.339 \text{ Mg m}^{-3} \)
\( \mu = 0.08 \text{ mm}^{-1} \)
\( T = 173 (2) \) K
Plate, light yellow
0.42 x 0.37 x 0.13 mm

Data collection
STOE IPDS II two-circle
diffractometer
0/2 scans
Absorption correction: none
9309 measured reflections
2940 independent reflections
2455 reflections with
I > 2\sigma(I)
\( R_{int} = 0.035 \)
\( \theta_{max} = 25.0 \)°

Refinement
Refinement on \( F^2 \)
\( wR(F^2) = 0.036 \)
\( S = 1.05 \)
2940 reflections
237 parameters
H-atom parameters constrained

H atoms were found in a difference map, but were positioned
g eo metrically and allowed to ride on their parent C atoms at
distances of 0.95 and 0.98 \( \text{Å} \) for \( sp^2 \) and methyl groups, respectively,
and with \( U_{eq} (H) = 1.2U_{eq} (C) \) or \( U_{eq} (H) = 1.5U_{eq} (C_{\text{methyl}}) \). 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, 1997); 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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