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4-Isopropyl-2-(4-methoxybenzylidene)-3,4-dihydronaphthalen-1(2*H*)-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.105
Data-to-parameter ratio = 15.0

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

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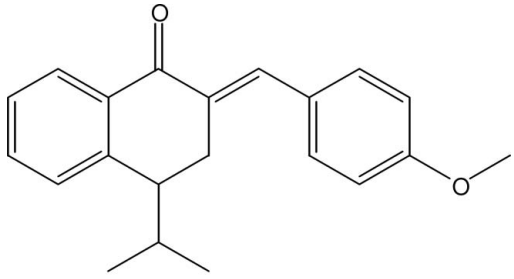
The title compound, $C_{21}H_{22}O_2$, has the exocyclic C=C double bond in an *E* configuration. The isopropyl group is attached in an axial position to the cyclohexenone ring.

Comment

Knowledge of the configuration and conformation of the title compound, (I), is necessary to understand its behaviour in dipolar-1,3 cycloaddition reactions (Badri *et al.*, 1999; Bennani *et al.*, 2002). To confirm the *E* configuration of the exocyclic C=C double bond and the axial position of the isopropyl group an X-ray crystal structure determination was carried out.



(I)

A perspective view of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Crystallographic Database, Version 1.7; Mogul Version 1.0.1; Allen, 2002). The exocyclic C=C double bond shows an *E* configuration. The carbonyl group is almost coplanar with this double bond [O1—C1—C2—C11 = −4.61 (18)°], but the *p*-methoxyphenyl ring attached to it is twisted out of the plane of the double bond [C2—C11—C12—C17 = −35.39 (19)°]. The isopropyl group is attached in an axial position to the cyclohexenone ring.

Experimental

The synthesis of 4-isopropyl-*para*-anisyl-phenylidene-2-tetralone-1 was achieved using the method reported by Kerbal *et al.* (1988), *i.e.* by a condensation of *para*-anisaldahyde with 4-isopropyltetralone-1 in an alkaline medium in methanol.

Crystal data

$C_{21}H_{22}O_2$
M_r = 306.39
Monoclinic, $P2_1/n$
a = 7.9380 (5) Å
b = 9.3745 (4) Å
c = 22.7340 (16) Å
β = 98.219 (5)°
V = 1674.37 (17) Å^3
Z = 4
D_x = 1.215 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25892 reflections
θ = 3.4–25.8°
μ = 0.08 mm^{-1}
T = 173 (2) K
Block, colourless
0.35 × 0.33 × 0.29 mm

Data collection

Stoe IPDS-II two-circle diffractometer	2800 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.040$
Absorption correction: none	$\theta_{max} = 25.6^\circ$
26652 measured reflections	$h = -9 \rightarrow 9$
3147 independent reflections	$k = -11 \rightarrow 11$
	$l = -27 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.4741P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.105$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
3147 reflections	Extinction correction: *SHELXL97*
210 parameters	Extinction coefficient: 0.024 (3)
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

O1—C1	1.2332 (15)	C2—C11	1.3458 (17)
C1—C2	1.4967 (17)	C11—C12	1.4703 (17)

All H atoms were located in a difference map and were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C_{methyl})] using a riding model, with C—H ranging from 0.95 to 1.00 Å. In addition, the CH_3 group attached to the O atom was 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: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

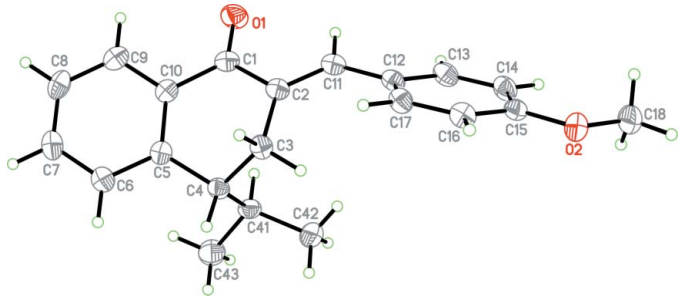


Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

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