Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-2-(4-Chlorobenzylidene)indan-1-one

Mohamed Ashraf Ali,[a] Tan Soo Choon,[a] Lim Yee Lan,[b] Mohd Mustaqim Rosli[c] and Hoong-Kun Fun[c]*‡

[a]Institute for Research in Molecular Medicine, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]School of Chemical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hkfun@usm.my

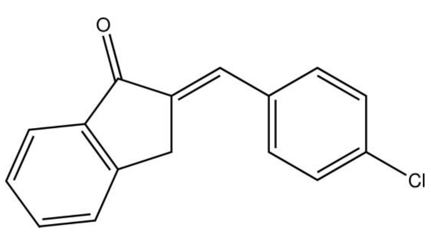
Received 22 June 2011; accepted 9 July 2011

Key indicators: single-crystal X-ray study; *T* = 100 K; mean σ(C–C) = 0.005 Å; *R* factor = 0.046; *wR* factor = 0.124; data-to-parameter ratio = 13.2.

In the title compound, $C_{16}H_{11}ClO$, the dihedral angle between the almost planar dihydroindene ring system (r.m.s. deviation = 0.009 Å) and the chlorobenzene ring is 3.51 (14)°. In the crystal, molecules are connected by C—H···O and weak C—H···Cl interactions, forming infinite layers parallel to (101).

Related literature

For biological background to dihydroindene derivatives, see: Akritopoulou-Zanze *et al.* (2007); Muhsin *et al.* (2006). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{16}H_{11}ClO$
M_r = 254.70
Triclinic, *P*1
a = 3.8649 (2) Å
b = 6.5233 (3) Å
c = 12.1703 (6) Å
α = 91.374 (4)°
β = 95.914 (4)°
γ = 103.483 (4)°
V = 296.43 (3) $Å^3$
Z = 1
Mo *K*α radiation
μ = 0.30 mm^{-1}
T = 100 K
0.43 × 0.28 × 0.04 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.882, T_{max} = 0.988
3942 measured reflections
2159 independent reflections
2072 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.124
S = 1.06
2159 reflections
163 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.48 e $Å^{-3}$
Absolute structure: Flack (1983), 870 Friedel pairs
Flack parameter: 0.05 (8)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O1^{i}	0.99	2.49	3.436 (4)	159
C5—H5*A*···Cl1^{ii}	0.95	2.80	3.591 (4)	141

Symmetry codes: (i) *x*, *y* − 1, *z*; (ii) *x* − 1, *y* + 1, *z* − 1.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

The authors wish to express their thanks to Universiti Sains Malaysia (USM), Penang, Malaysia for providing research facilities. HKF also thanks USM for the Research University Grant (No. 1001/PFIZIK/811160).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5928).

References

Akritopoulou-Zanze, I., Albert, D. H., Bousquet, P. F., Cunha, G. A., Harris, C. M., Moskey, M., Dinges, J., Stewart, K. D. & Sowin, T. J. (2007). *Bioorg. Med. Chem. Lett.* **17**, 3136–3140.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Muhsin, M., Graham, J. & Kirkpatrick, P. (2006). *Nat. Rev. Drug Disc.* **3**, 995–996.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

‡ Thomson Reuters ResearcherID: A-3561-2009.

supplementary materials

Acta Cryst. (2011). E**67**, o2064 [**doi:10.1107/S1600536811027589**]

(*E*)-2-(4-Chlorobenzylidene)indan-1-one

M. A. Ali, T. S. Choon, L. Y. Lan, M. M. Rosli and H.-K. Fun

Comment

Substituted dihydroindene derivatives have been used as multitargeted kinase inhibitors: Initial efforts focused on the development of selective KDR inhibitors, while later strategies involved the improvement of potency toward multiple kinase targets (Akritopoulou-Zanze *et al.* 2007). Thus, several dihydroindene derivatives were identified as potent KDR, Flt1, Flt3, and c-Kit inhibitors. Initial strategies involved single target therapies and resulted in the FDA approval of Avastin (a humanized monoclonal antibody targeting VEGF, the growth factor that stimulates VEGFRs) for the treatment of metastatic colorectal cancer (Muhsin *et al.* 2006). As part of our studies in this area, we now report the synthesis and structure of the title compound, (I).

All parameters in (I) within normal ranges. The dihydroindene ring is almost planar with the maximum deviation of -0.015 (4)Å for atom C7. It make a dihedral angle of 3.51 (14)° with the adjacent benzene ring (Fig. 1). In the crystal, the molecules are interconnected by C—H···O and C—H···Cl interactions (Table 1) to form infinite layers (Fig. 2) parallel to the (101)-plane.

Experimental

A mixture of 2,3-dihydro-IH-indene-1-one (0.001 mmol) and 4-chlorbenzaldehyde (0.001 mmol) were dissolved in methanol (10 mL) and 30% sodium hydroxide solution (5ml) was added. The solution was stirred for 5 hour. After completion of the reaction as evident from TLC, the mixture was poured into crushed ice then neutralized with Con HCl. The precipitated solid was filtered, washed with water and recrystallised from ethanol to reveal the title compound as light yellow plates of (I).

Refinement

All H-atoms were positioned geometrically and refined using a riding model, with C-H = 0.95 and 0.99Å, and with $U_{iso} = 1.2U_{eq}(C)$.

Figures

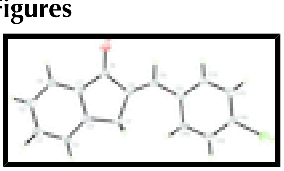


Fig. 1. The molecular structure, showing 50% probability displacement ellipsoids. Hydrogen atoms are shown as spheres of arbitrary radius.

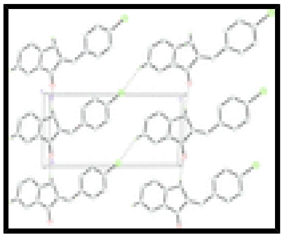


Fig. 2. The packing of (I) viewed along the a axis. Dashed lines indicate hydrogen bonds. H atoms not involved in the hydrogen bond interactions have been omitted for clarity.

(*E*)-2-(4-Chlorobenzylidene)indan-1-one

Crystal data

$C_{16}H_{11}ClO$	$Z = 1$
$M_r = 254.70$	$F(000) = 132$
Triclinic, *P*1	$D_x = 1.427$ Mg m^{-3}
Hall symbol: P 1	Mo *K*α radiation, λ = 0.71073 Å
a = 3.8649 (2) Å	Cell parameters from 2756 reflections
b = 6.5233 (3) Å	θ = 3.2–32.1°
c = 12.1703 (6) Å	μ = 0.30 mm^{-1}
α = 91.374 (4)°	*T* = 100 K
β = 95.914 (4)°	Plate, light-yellow
γ = 103.483 (4)°	0.43 × 0.28 × 0.04 mm
V = 296.43 (3) Å^3	

Data collection

Bruker SMART APEXII CCD diffractometer	2159 independent reflections
Radiation source: fine-focus sealed tube	2072 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.039$
φ and ω scans	$\theta_{max} = 27.0°$, $\theta_{min} = 1.7°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$h = -4 \rightarrow 4$
$T_{min} = 0.882$, $T_{max} = 0.988$	$k = -8 \rightarrow 8$
3942 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.124$	$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 0.1711P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
2159 reflections	$\Delta\rho_{max} = 0.63$ e Å^{-3}
163 parameters	$\Delta\rho_{min} = -0.48$ e Å^{-3}

3 restraints	Absolute structure: Flack (1983), 870 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.05 (8)

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.33869 (16)	−0.02880 (10)	0.53352 (7)	0.0254 (2)
O1	0.9589 (7)	0.8574 (3)	0.0177 (2)	0.0249 (5)
C1	0.5969 (8)	0.2910 (5)	0.0183 (3)	0.0179 (7)
H1A	0.7420	0.1882	0.0046	0.022*
H1B	0.4062	0.2263	0.0639	0.022*
C2	0.4406 (9)	0.3621 (5)	−0.0892 (3)	0.0184 (6)
C3	0.2093 (9)	0.2374 (5)	−0.1742 (3)	0.0194 (7)
H3A	0.1294	0.0893	−0.1683	0.023*
C4	0.0999 (9)	0.3344 (5)	−0.2667 (3)	0.0226 (7)
H4A	−0.0572	0.2512	−0.3248	0.027*
C5	0.2154 (10)	0.5534 (6)	−0.2770 (3)	0.0239 (7)
H5A	0.1358	0.6175	−0.3410	0.029*
C6	0.4483 (9)	0.6754 (5)	−0.1921 (3)	0.0221 (7)
H6A	0.5322	0.8231	−0.1983	0.026*
C7	0.5554 (9)	0.5799 (5)	−0.0994 (3)	0.0196 (7)
C8	0.8022 (8)	0.6717 (5)	−0.0003 (3)	0.0186 (7)
C9	0.8293 (9)	0.4952 (5)	0.0738 (3)	0.0188 (7)
C10	1.0366 (9)	0.5332 (5)	0.1708 (3)	0.0195 (7)
H10A	1.1649	0.6758	0.1856	0.023*
C11	1.0966 (8)	0.3896 (5)	0.2575 (3)	0.0177 (7)
C12	1.3093 (9)	0.4750 (5)	0.3561 (3)	0.0205 (7)
H12A	1.4065	0.6231	0.3639	0.025*
C13	1.3816 (9)	0.3519 (6)	0.4415 (3)	0.0225 (7)
H13A	1.5242	0.4136	0.5076	0.027*
C14	1.2417 (9)	0.1354 (5)	0.4291 (3)	0.0202 (7)
C15	1.0307 (9)	0.0433 (5)	0.3330 (3)	0.0210 (7)
H15A	0.9361	−0.1051	0.3259	0.025*
C16	0.9595 (9)	0.1698 (5)	0.2477 (3)	0.0178 (7)

H16A	0.8164	0.1071	0.1818	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0283 (4)	0.0188 (4)	0.0279 (4)	0.0036 (3)	0.0010 (3)	0.0050 (3)
O1	0.0255 (13)	0.0120 (11)	0.0341 (13)	−0.0017 (10)	0.0027 (10)	0.0018 (9)
C1	0.0187 (16)	0.0079 (13)	0.0265 (16)	−0.0002 (12)	0.0066 (13)	0.0009 (11)
C2	0.0165 (16)	0.0129 (14)	0.0253 (15)	0.0011 (13)	0.0048 (12)	0.0038 (12)
C3	0.0150 (15)	0.0120 (15)	0.0273 (17)	−0.0045 (13)	0.0025 (13)	−0.0001 (12)
C4	0.0166 (16)	0.0209 (16)	0.0263 (16)	−0.0032 (14)	0.0017 (13)	−0.0013 (13)
C5	0.0201 (17)	0.0222 (18)	0.0279 (17)	0.0004 (14)	0.0046 (13)	0.0051 (13)
C6	0.0204 (17)	0.0136 (15)	0.0311 (18)	0.0006 (13)	0.0051 (14)	0.0042 (12)
C7	0.0161 (16)	0.0139 (15)	0.0272 (17)	−0.0006 (12)	0.0052 (13)	−0.0006 (12)
C8	0.0148 (15)	0.0118 (14)	0.0297 (17)	0.0024 (12)	0.0053 (13)	0.0037 (12)
C9	0.0163 (15)	0.0092 (15)	0.0293 (17)	−0.0019 (12)	0.0064 (13)	0.0006 (12)
C10	0.0180 (16)	0.0102 (14)	0.0276 (16)	−0.0023 (12)	0.0031 (13)	0.0005 (12)
C11	0.0146 (16)	0.0121 (15)	0.0262 (17)	0.0021 (12)	0.0040 (13)	0.0006 (12)
C12	0.0181 (16)	0.0131 (15)	0.0283 (17)	0.0003 (13)	0.0015 (13)	−0.0033 (12)
C13	0.0171 (17)	0.0207 (17)	0.0273 (18)	0.0001 (14)	0.0025 (14)	−0.0039 (14)
C14	0.0159 (17)	0.0200 (17)	0.0251 (17)	0.0037 (13)	0.0039 (13)	0.0088 (13)
C15	0.0209 (18)	0.0147 (16)	0.0270 (18)	0.0031 (14)	0.0030 (14)	0.0017 (13)
C16	0.0165 (16)	0.0111 (15)	0.0232 (17)	−0.0012 (13)	0.0014 (13)	0.0000 (12)

Geometric parameters (Å, °)

Cl1—C14	1.749 (3)	C7—C8	1.478 (5)
O1—C8	1.225 (4)	C8—C9	1.495 (4)
C1—C2	1.513 (5)	C9—C10	1.340 (5)
C1—C9	1.520 (4)	C10—C11	1.464 (5)
C1—H1A	0.9900	C10—H10A	0.9500
C1—H1B	0.9900	C11—C12	1.405 (4)
C2—C7	1.399 (4)	C11—C16	1.406 (4)
C2—C3	1.400 (4)	C12—C13	1.375 (5)
C3—C4	1.382 (5)	C12—H12A	0.9500
C3—H3A	0.9500	C13—C14	1.388 (5)
C4—C5	1.407 (5)	C13—H13A	0.9500
C4—H4A	0.9500	C14—C15	1.391 (5)
C5—C6	1.395 (5)	C15—C16	1.386 (5)
C5—H5A	0.9500	C15—H15A	0.9500
C6—C7	1.375 (5)	C16—H16A	0.9500
C6—H6A	0.9500		
C2—C1—C9	103.1 (3)	C7—C8—C9	107.3 (3)
C2—C1—H1A	111.2	C10—C9—C8	120.3 (3)
C9—C1—H1A	111.2	C10—C9—C1	131.1 (3)
C2—C1—H1B	111.2	C8—C9—C1	108.5 (3)
C9—C1—H1B	111.2	C9—C10—C11	130.2 (3)
H1A—C1—H1B	109.1	C9—C10—H10A	114.9

C7—C2—C3	119.8 (3)	C11—C10—H10A	114.9
C7—C2—C1	112.3 (3)	C12—C11—C16	117.6 (3)
C3—C2—C1	127.8 (3)	C12—C11—C10	118.4 (3)
C4—C3—C2	118.6 (3)	C16—C11—C10	124.0 (3)
C4—C3—H3A	120.7	C13—C12—C11	122.4 (3)
C2—C3—H3A	120.7	C13—C12—H12A	118.8
C3—C4—C5	121.6 (3)	C11—C12—H12A	118.8
C3—C4—H4A	119.2	C12—C13—C14	118.5 (3)
C5—C4—H4A	119.2	C12—C13—H13A	120.8
C6—C5—C4	119.2 (3)	C14—C13—H13A	120.8
C6—C5—H5A	120.4	C13—C14—C15	121.3 (3)
C4—C5—H5A	120.4	C13—C14—Cl1	120.2 (2)
C7—C6—C5	119.4 (3)	C15—C14—Cl1	118.5 (3)
C7—C6—H6A	120.3	C16—C15—C14	119.5 (3)
C5—C6—H6A	120.3	C16—C15—H15A	120.3
C6—C7—C2	121.3 (3)	C14—C15—H15A	120.3
C6—C7—C8	129.9 (3)	C15—C16—C11	120.7 (3)
C2—C7—C8	108.7 (3)	C15—C16—H16A	119.6
O1—C8—C7	126.5 (3)	C11—C16—H16A	119.6
O1—C8—C9	126.1 (3)		

C9—C1—C2—C7	−0.5 (4)	O1—C8—C9—C1	−178.8 (3)
C9—C1—C2—C3	178.9 (3)	C7—C8—C9—C1	0.6 (3)
C7—C2—C3—C4	0.0 (5)	C2—C1—C9—C10	−179.6 (3)
C1—C2—C3—C4	−179.4 (3)	C2—C1—C9—C8	−0.1 (3)
C2—C3—C4—C5	0.0 (5)	C8—C9—C10—C11	177.9 (3)
C3—C4—C5—C6	0.5 (5)	C1—C9—C10—C11	−2.6 (6)
C4—C5—C6—C7	−1.1 (5)	C9—C10—C11—C12	−175.1 (3)
C5—C6—C7—C2	1.2 (5)	C9—C10—C11—C16	6.1 (6)
C5—C6—C7—C8	178.7 (3)	C16—C11—C12—C13	−0.7 (5)
C3—C2—C7—C6	−0.6 (5)	C10—C11—C12—C13	−179.6 (3)
C1—C2—C7—C6	178.9 (3)	C11—C12—C13—C14	0.7 (5)
C3—C2—C7—C8	−178.6 (3)	C12—C13—C14—C15	−0.4 (5)
C1—C2—C7—C8	0.9 (4)	C12—C13—C14—Cl1	177.8 (3)
C6—C7—C8—O1	0.7 (5)	C13—C14—C15—C16	0.3 (5)
C2—C7—C8—O1	178.5 (3)	Cl1—C14—C15—C16	−178.0 (3)
C6—C7—C8—C9	−178.6 (3)	C14—C15—C16—C11	−0.3 (5)
C2—C7—C8—C9	−0.9 (4)	C12—C11—C16—C15	0.5 (5)
O1—C8—C9—C10	0.8 (5)	C10—C11—C16—C15	179.3 (3)
C7—C8—C9—C10	−179.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1A···O1^{i}	0.99	2.49	3.436 (4)	159
C5—H5A···Cl1^{ii}	0.95	2.80	3.591 (4)	141

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*−1, *y*+1, *z*−1.

Fig. 1

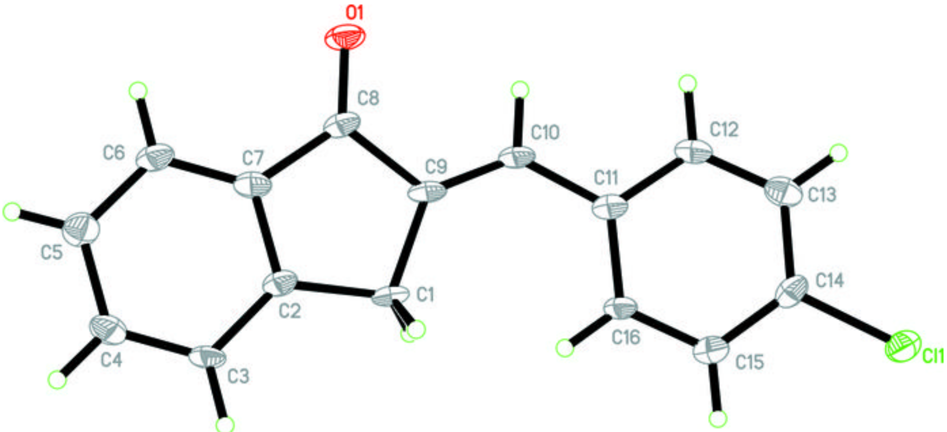


Fig. 2