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(*E*)-1-[(3-Iodophenyl)iminomethyl]-naphthalen-2-ol

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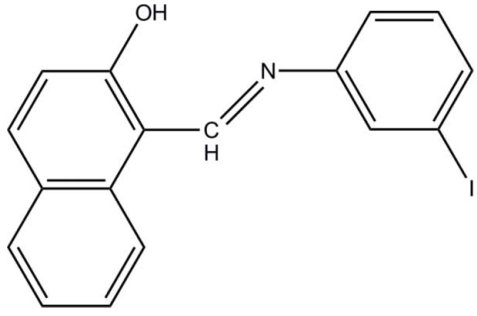
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.008 Å; R factor = 0.042; wR factor = 0.094; data-to-parameter ratio = 15.4.

In the title molecule, $C_{17}H_{12}INO$, the dihedral angle between the naphthaldeyde plane and the 3-iodoaniline plane is20.07 (13)°. It exists in the solid state as an enol–imine tautomer with a strong intramolecular O—H···N hydrogen bond.

Related literature

For the applications of iodoaromatic compounds in synthetic organic chemistry, medicine and biochemistry, see; Merkushev (1988); Olah *et al.* (1993). Schiff base complexes have been used in catalytic reactions and are used as models for biological systems, see: Hamilton *et al.* (1987); Pyrz *et al.* (1985); Costamagna *et al.* (1992). For related structures, see: Ünver *et al.* (2000); Manvizhi *et al.* (2011).



Experimental

Crystal data

$C_{17}H_{12}INO$ M_r = 373.18
Monoclinic, $C2/c$
a = 32.059 (3) Å
b = 4.8392 (3) Å
c = 19.2682 (16) Å
β = 107.269 (6)°
V = 2854.5 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.24 mm^{-1}
T = 296 K
0.80 × 0.30 × 0.03 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.793, T_{max} = 0.925
9569 measured reflections
2781 independent reflections
1607 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.094
S = 0.93
2781 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.82	2.555 (6)	148

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *WinGX* (Farrugia, 1997) and *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2093).

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(*E*)-1-[(3-Iodophenyl)iminomethyl]naphthalen-2-ol

Tufan Akbal, Ayşen Ağar Alaman, Sümeyye Gümüş and Ahmet Erdönmez

S1. Comment

Iodoaromatic compounds are valuable and versatile synthetic intermediates in many domains of synthetic organic chemistry, medicine and biochemistry (Merkushev *et al.*, 1988; Olah *et al.*, 1993). The Schiff base complexes have also been used in catalytic reactions (Hamilton *et al.*, 1987) are used as models for biological systems (Pyrz *et al.*, 1985; Costamagna *et al.*, 1992). There are two types of intramolecular hydrogen bonds in Schiff bases, namely keto-amine (N—H···O) and enol-imine (N···H—O) tautomeric forms. The present X-ray investigation shows that the title compound,(I), prefers the enol-imine tautomeric form rather than the keto-amine tautomeric form. The C9—O1 and C7—N1 bond lengths verify the enol-imine tautomeric form. these distances agree with the literature[1.310 (8) and 1.319 (6)Â; Ünver *et al.* 2000], which also show the enol-imine tautomeric form. The C1—I1 bond lenght in (I) is also in a good agremeent with the corresponding distances in the literature [2.092 (4)Â; Manvizhi *et al.*, 2011]. The bond distances for O1-H1O1 and N1-H1O1 are 0.82 and 1.82 Â, respectively, and the N1···H1—O1 angle is 148 Å. These distances and angle agree with the literature[Ünver *et al.* 2000], The title molecule with the atom-numbering scheme. The displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond. An *ORTEP-3* (Farrugia, 1997) packing diagram of (I), viewed along the *b* axis. The molecule is non-planar. The angle between the two Schiff base moieties [C1—C6,N1,I1] and [C7—C13,O1,N1] is 20.07 (13) Å. *Cg*(1), *Cg*(2) and *Cg*(3) are the centroids of rings C1—C6, C8—C13 and C12—C17, respectively. However, $\pi\cdots\pi$ interactions between the centroids of the *Cg*(1) and *Cg*(2) rings (distance between ring centroids = 4.664 (3) Â), and the *Cg*(2) and *Cg*(3) rings (distance between ring centroids = 4.791 (3)Â), stack the molecules along the *b*-axis.

S2. Experimental

The compound *E*)—*1*-((3-iodophenyllimino)methyl)naphthalen-2-ol (*E*)-1-((3-bromophenyllimino)methyl)naphthalen-2-ol was prepared by refluxing a mixture of a solution containing 2-hydroxy-1-naphthaldehyde (17.2 mg 0.100 mmol) in 30 ml absolute ethanol and a solution containing 3-iodoaniline (21.9 mg 0.100 mmol) in 20 ml absolute ethanol. The reaction mixture was stirred for 4 h under reflux. Single crystals of the title compound for X-ray anaysis were obtaned by slow evaporation of an ethaol solition (yield % 67; m.p 410–412 ^{o}K).

S3. Refinement

All carbon attached H-atoms were refined using riding model for hydrogen bonds with d(C—H) = 0.93 Å (U_{iso}=1.2U_{eq} of the parent atom) for aromatic carbon atoms and d(C—H) = 0.96 Å (U_{iso}=1.5U_{eq} of the parent atom) for methyl carbon atoms.

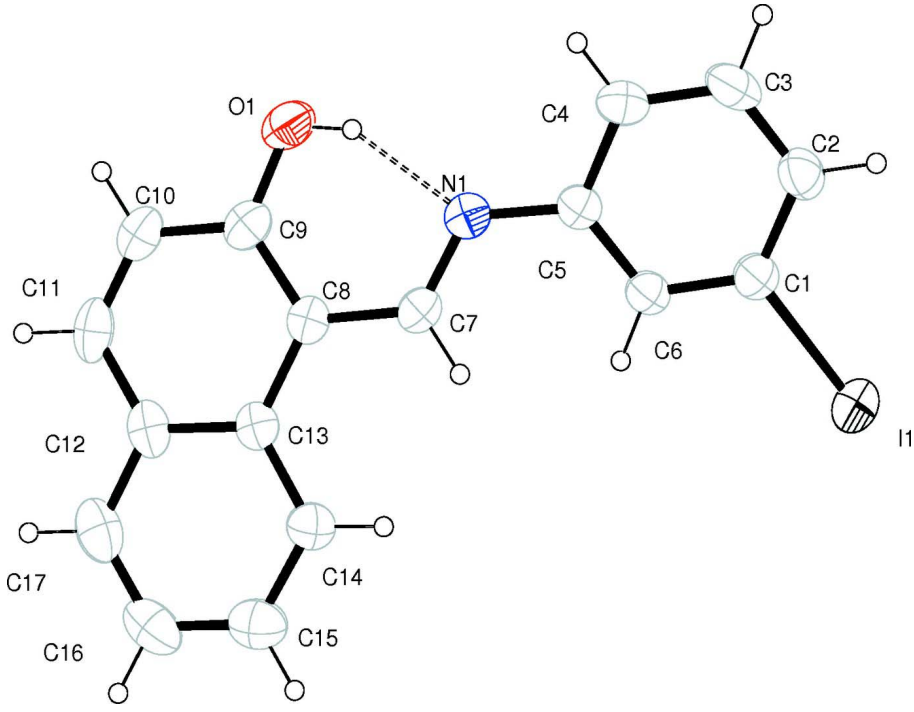

Figure 1

The title molecule with the atom-numbering scheme. The displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond.

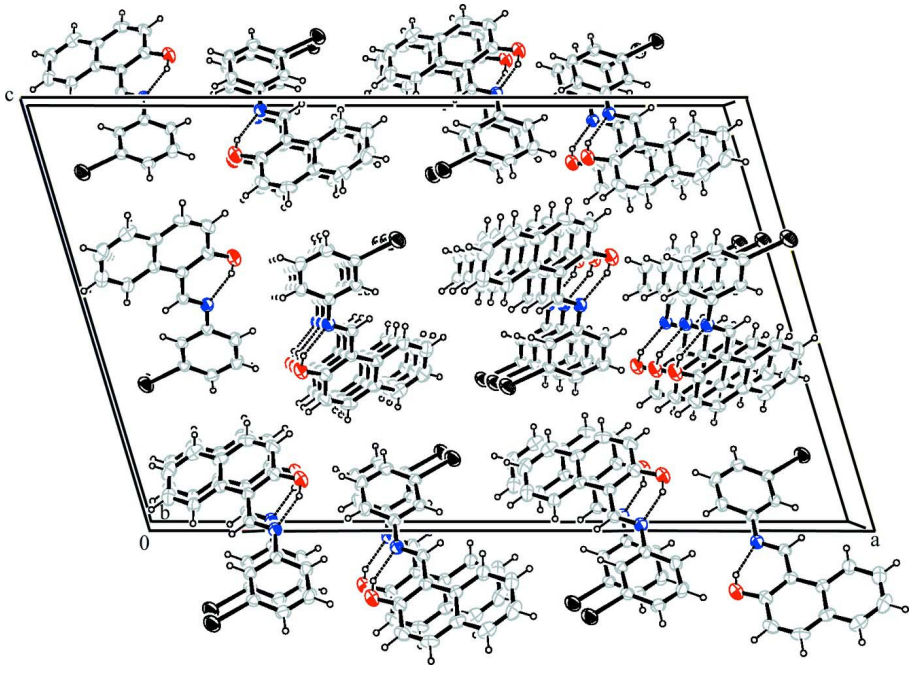

Figure 2

An *ORTEP-3* (Farrugia, 1997) packing diagram of (I), viewed along the *b* axis.

(*E*)-1-[(3-Iodophenyl)iminomethyl]naphthalen-2-ol

Crystal data

$C_{17}H_{12}INO$
$M_r = 373.18$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 32.059$ (3) Å
$b = 4.8392$ (3) Å
$c = 19.2682$ (16) Å
$\beta = 107.269$ (6)°
$V = 2854.5$ (4) Å^3
$Z = 8$
$F(000) = 1456$
$D_x = 1.737$ Mg m^{-3}
Melting point = 410–412 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9569 reflections
$\theta = 1.3$–$26.0°$
$\mu = 2.24$ mm^{-1}
$T = 296$ K
Needle, yellow
0.80 × 0.30 × 0.03 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
w–scan rotation
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.793$, $T_{max} = 0.925$
9569 measured reflections
2781 independent reflections
1607 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.3°$
$h = -38 \rightarrow 38$
$k = -5 \rightarrow 5$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.094$
$S = 0.93$
2781 reflections
181 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.87$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008)
Extinction coefficient: 0

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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}
I1	0.052729 (12)	0.52255 (9)	0.33319 (2)	0.08465 (19)
C5	0.16216 (15)	0.0503 (9)	0.4653 (2)	0.0490 (11)

C8	0.15014 (14)	−0.4836 (10)	0.5955 (2)	0.0498 (11)
O1	0.22667 (12)	−0.3804 (8)	0.6294 (2)	0.0784 (11)
H1	0.2177	−0.2766	0.5946	0.118*
C9	0.19336 (16)	−0.5200 (11)	0.6398 (3)	0.0593 (13)
C11	0.1710 (2)	−0.8587 (12)	0.7108 (3)	0.0712 (16)
H11	0.1781	−0.9838	0.7491	0.085*
N1	0.17155 (13)	−0.1458 (9)	0.5220 (2)	0.0546 (10)
C4	0.19651 (17)	0.1402 (12)	0.4410 (3)	0.0620 (13)
H4	0.2243	0.0672	0.4616	0.074*
C6	0.12123 (16)	0.1594 (10)	0.4331 (2)	0.0514 (12)
H6	0.0976	0.1010	0.4481	0.062*
C7	0.14134 (16)	−0.2876 (10)	0.5375 (2)	0.0508 (12)
H7	0.1125	−0.2607	0.5096	0.061*
C3	0.19005 (19)	0.3351 (13)	0.3873 (3)	0.0721 (16)
H3	0.2135	0.3935	0.3720	0.087*
C2	0.14946 (18)	0.4450 (11)	0.3557 (3)	0.0655 (14)
H2	0.1451	0.5779	0.3194	0.079*
C1	0.11518 (16)	0.3532 (11)	0.3793 (2)	0.0544 (12)
C13	0.11570 (16)	−0.6479 (10)	0.6093 (2)	0.0510 (12)
C17	0.0936 (2)	−0.9958 (12)	0.6815 (3)	0.0797 (16)
H17	0.1007	−1.1192	0.7203	0.096*
C14	0.07180 (17)	−0.6311 (12)	0.5668 (3)	0.0651 (14)
H14	0.0638	−0.5092	0.5277	0.078*
C16	0.0511 (2)	−0.9750 (14)	0.6391 (4)	0.0868 (18)
H16	0.0296	−1.0836	0.6488	0.104*
C10	0.20262 (19)	−0.7080 (12)	0.6980 (3)	0.0693 (15)
H10	0.2312	−0.7273	0.7279	0.083*
C12	0.1268 (2)	−0.8351 (11)	0.6679 (3)	0.0613 (14)
C15	0.0407 (2)	−0.7938 (14)	0.5825 (4)	0.0810 (17)
H15	0.0118	−0.7799	0.5538	0.097*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0709 (2)	0.0937 (3)	0.0771 (3)	0.0026 (2)	0.00310 (19)	0.0215 (2)
C5	0.053 (3)	0.047 (3)	0.047 (3)	−0.006 (2)	0.014 (2)	−0.009 (2)
C8	0.058 (3)	0.048 (3)	0.045 (2)	0.007 (2)	0.017 (2)	−0.005 (2)
O1	0.054 (2)	0.094 (3)	0.079 (3)	0.005 (2)	0.007 (2)	0.005 (2)
C9	0.058 (3)	0.060 (3)	0.058 (3)	0.010 (3)	0.015 (2)	−0.010 (3)
C11	0.104 (5)	0.060 (4)	0.045 (3)	0.021 (3)	0.014 (3)	0.006 (3)
N1	0.053 (2)	0.055 (3)	0.056 (2)	0.001 (2)	0.016 (2)	−0.005 (2)
C4	0.053 (3)	0.067 (4)	0.067 (3)	−0.011 (3)	0.019 (3)	−0.009 (3)
C6	0.054 (3)	0.056 (3)	0.045 (3)	−0.010 (2)	0.015 (2)	−0.005 (2)
C7	0.050 (3)	0.053 (3)	0.046 (3)	0.004 (2)	0.010 (2)	−0.007 (2)
C3	0.069 (4)	0.085 (4)	0.070 (4)	−0.027 (3)	0.032 (3)	−0.004 (3)
C2	0.073 (3)	0.073 (4)	0.051 (3)	−0.012 (3)	0.018 (3)	0.004 (3)
C1	0.058 (3)	0.060 (3)	0.043 (3)	−0.009 (2)	0.011 (2)	−0.007 (2)
C13	0.060 (3)	0.045 (3)	0.052 (3)	0.005 (2)	0.022 (2)	−0.007 (2)

C17	0.114 (5)	0.059 (4)	0.080 (4)	0.007 (4)	0.049 (4)	0.005 (3)
C14	0.059 (3)	0.068 (4)	0.070 (3)	−0.002 (3)	0.022 (3)	0.001 (3)
C16	0.099 (5)	0.073 (4)	0.107 (5)	−0.017 (4)	0.059 (4)	−0.005 (4)
C10	0.067 (4)	0.071 (4)	0.060 (3)	0.014 (3)	0.004 (3)	0.001 (3)
C12	0.090 (4)	0.048 (3)	0.053 (3)	0.008 (3)	0.032 (3)	−0.001 (2)
C15	0.069 (4)	0.082 (5)	0.097 (5)	−0.006 (3)	0.032 (4)	−0.013 (4)

Geometric parameters (Å, º)

I1—C1	2.101 (5)	C6—H6	0.9300
C5—C6	1.379 (6)	C7—H7	0.9300
C5—C4	1.387 (6)	C3—C2	1.370 (7)
C5—N1	1.411 (6)	C3—H3	0.9300
C8—C9	1.406 (6)	C2—C1	1.381 (7)
C8—C7	1.428 (6)	C2—H2	0.9300
C8—C13	1.448 (7)	C13—C14	1.406 (7)
O1—C9	1.328 (6)	C13—C12	1.408 (7)
O1—H1	0.8200	C17—C16	1.368 (9)
C9—C10	1.405 (7)	C17—C12	1.404 (8)
C11—C10	1.331 (8)	C17—H17	0.9300
C11—C12	1.416 (7)	C14—C15	1.373 (8)
C11—H11	0.9300	C14—H14	0.9300
N1—C7	1.292 (6)	C16—C15	1.361 (9)
C4—C3	1.370 (8)	C16—H16	0.9300
C4—H4	0.9300	C10—H10	0.9300
C6—C1	1.369 (7)	C15—H15	0.9300
C6—C5—C4	118.3 (5)	C3—C2—H2	120.9
C6—C5—N1	124.1 (4)	C1—C2—H2	120.9
C4—C5—N1	117.6 (4)	C6—C1—C2	121.4 (5)
C9—C8—C7	119.3 (4)	C6—C1—I1	119.4 (4)
C9—C8—C13	119.1 (4)	C2—C1—I1	119.2 (4)
C7—C8—C13	121.6 (4)	C14—C13—C12	118.4 (5)
C9—O1—H1	109.5	C14—C13—C8	123.1 (4)
O1—C9—C10	117.4 (5)	C12—C13—C8	118.4 (5)
O1—C9—C8	122.4 (5)	C16—C17—C12	121.5 (6)
C10—C9—C8	120.2 (5)	C16—C17—H17	119.2
C10—C11—C12	122.2 (5)	C12—C17—H17	119.2
C10—C11—H11	118.9	C15—C14—C13	120.3 (5)
C12—C11—H11	118.9	C15—C14—H14	119.9
C7—N1—C5	122.3 (4)	C13—C14—H14	119.9
C3—C4—C5	120.9 (5)	C15—C16—C17	119.3 (6)
C3—C4—H4	119.6	C15—C16—H16	120.4
C5—C4—H4	119.6	C17—C16—H16	120.4
C1—C6—C5	120.3 (4)	C11—C10—C9	120.7 (5)
C1—C6—H6	119.8	C11—C10—H10	119.7
C5—C6—H6	119.8	C9—C10—H10	119.7
N1—C7—C8	123.1 (4)	C17—C12—C13	118.8 (6)

N1—C7—H7	118.5	C17—C12—C11	121.9 (5)
C8—C7—H7	118.5	C13—C12—C11	119.4 (5)
C2—C3—C4	120.9 (5)	C16—C15—C14	121.7 (6)
C2—C3—H3	119.6	C16—C15—H15	119.1
C4—C3—H3	119.6	C14—C15—H15	119.1
C3—C2—C1	118.3 (5)		

C7—C8—C9—O1	−0.8 (7)	C7—C8—C13—C14	1.2 (7)
C13—C8—C9—O1	178.7 (4)	C9—C8—C13—C12	1.1 (6)
C7—C8—C9—C10	178.8 (4)	C7—C8—C13—C12	−179.4 (4)
C13—C8—C9—C10	−1.7 (7)	C12—C13—C14—C15	0.2 (8)
C6—C5—N1—C7	16.5 (7)	C8—C13—C14—C15	179.6 (5)
C4—C5—N1—C7	−164.2 (4)	C12—C17—C16—C15	−0.2 (9)
C6—C5—C4—C3	0.9 (7)	C12—C11—C10—C9	−1.1 (9)
N1—C5—C4—C3	−178.5 (4)	O1—C9—C10—C11	−178.7 (5)
C4—C5—C6—C1	−0.6 (7)	C8—C9—C10—C11	1.7 (8)
N1—C5—C6—C1	178.7 (4)	C16—C17—C12—C13	0.3 (8)
C5—N1—C7—C8	−179.0 (4)	C16—C17—C12—C11	−178.9 (5)
C9—C8—C7—N1	2.2 (7)	C14—C13—C12—C17	−0.3 (7)
C13—C8—C7—N1	−177.2 (4)	C8—C13—C12—C17	−179.8 (4)
C5—C4—C3—C2	−0.4 (8)	C14—C13—C12—C11	179.0 (5)
C4—C3—C2—C1	−0.3 (8)	C8—C13—C12—C11	−0.5 (7)
C5—C6—C1—C2	−0.1 (7)	C10—C11—C12—C17	179.7 (5)
C5—C6—C1—I1	−178.5 (3)	C10—C11—C12—C13	0.5 (8)
C3—C2—C1—C6	0.6 (8)	C17—C16—C15—C14	0.1 (9)
C3—C2—C1—I1	179.0 (4)	C13—C14—C15—C16	−0.1 (9)
C9—C8—C13—C14	−178.3 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.82	2.555 (6)	148