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2,4-Diiodo-6-{[4-(morpholin-4-yl)-phenyl]iminomethyl}phenol

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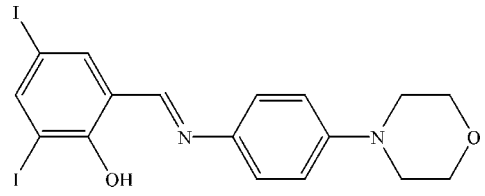
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.056; wR factor = 0.113; data-to-parameter ratio = 36.8.

In the title compound, $C_{17}H_{16}I_2N_2O_2$, the two aromatic rings are almost coplanar [dihedral angle 2.57 (15)°]. The morpholine ring adopts a chair conformation. The molecular structure is stabilized by an O—H···N hydrogen bond and the crystal packing exhibits weak intermolecular C—H···O and π–π [centroid-to-centroid distances 3.663 (3)-4.073 (3) Å] interactions.

Related literature

For the biological activity of morpholine derivatives, see: Lan *et al.* (2010); Raparti *et al.*(2009). For a related structure, see: Yang *et al.* (2011). For the definition of puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{17}H_{16}I_2N_2O_2$ M_r = 534.12
Monoclinic, $C2/c$
a = 26.4133 (16) Å
b = 7.6598 (4) Å
c = 18.0332 (11) Å
β = 91.417 (2)°
V = 3647.4 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.46 mm^{-1}
T = 295 K
0.26 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.467, T_{max} = 0.545
17839 measured reflections
7647 independent reflections
4855 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.113
S = 1.16
7647 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.22 e Å^{-3}
$\Delta\rho_{min}$ = −1.72 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1	0.82	1.82	2.548 (5)	146
C6—H6···O1^{i}	0.93	2.50	3.413 (5)	166

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5621).

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supporting information

Acta Cryst. (2011). E**67**, o2500 [doi:10.1107/S1600536811034519]

2,4-Diiodo-6-{[4-(morpholin-4-yl)phenyl]iminomethyl}phenol

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S1. Comment

Morpholine derivatives possess anticancer and antimicrobial (Lan *et al.*, 2010; Raparti *et al.*, 2009) activities. In the title compound, (I) (Fig. 1), The bond lengths C═N [1.282 (6)Å], C—I [C1—I1 = 2.092 (4) and C5—I2 = 2.097 (4) Å] are comparable with the literature values and the bond lengths of the morpholine ring are agree well with a reported related structure (Yang *et al.*, 2011).

The mean planes of two benzene rings (C8–C13) and (C1–C6) are oriented at an angle of 2.57 (15)°. The morpholine ring adopts a chair conformation [Puckering parameters are Q = 0.544 (6)Å, θ = 170.8 (5)° and φ = 180 (4)° (Cremer & Pople, 1975) for the ring (O1/C15/C14/N2/C17/C16)].

The molecular structure is stabilized by O—H···N hydrogen bonding and the crystal packing exhibit weak intermolecular C—H···O (Fig. 2 and Table 1) and π–π [Cg2···Cg3(-x, -y, -z) distance of 3.663 (3)Å; Cg2···Cg3(-x, 1 - y, -z) distance of 4.074 (3)Å] interactions.

S2. Experimental

An ethanolic solution (20 ml) of 4-(4-aminophenyl)morpholine (10 mmol) was magnetically stirred in a round bottom flask followed by drop wise addition of ethanolic solution of 3,5-diiodosalicylaldehyde (10 mmol). The reaction mixture was then refluxed for 3 h and upon cooling to 273 K, a red crystalline solid precipitates from the mixture. The solid which is separated out was filtered washed with ice cold ethanol and dried in vaccuo over anhydrous $CaCl_2$. Single crystals suitable for the X-ray diffraction were obtained by slow evaporation of a solution of the title compound in methanol at room temperature. m.p. 443 K.

S3. Refinement

All H atoms were positioned geometrically with C—H = 0.93–0.97 Å and O—H = 0.82 Å and allowed to ride on their parent atoms, with U_{iso}(H) = 1.5Ueq(O) and 1.2Ueq(C).

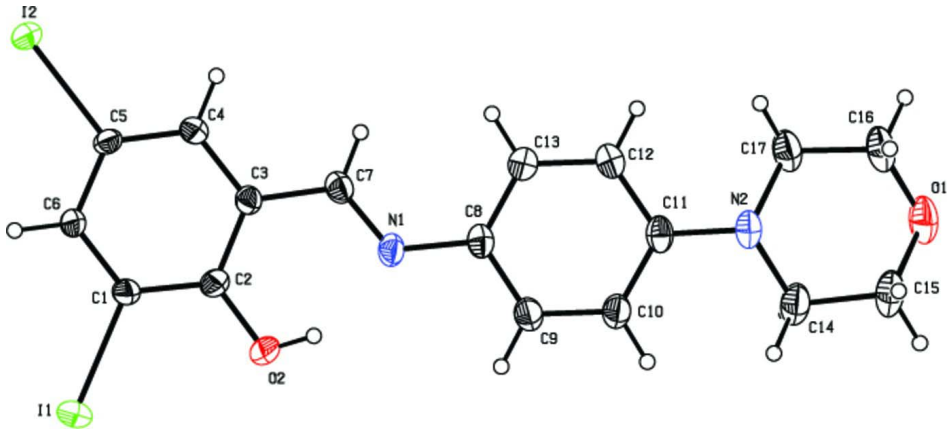

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

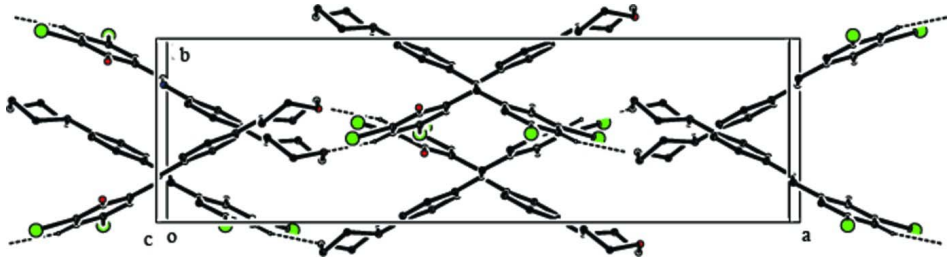

Figure 2

The packing of the title compound, viewed down the *c* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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Crystal data

$C_{17}H_{16}I_2N_2O_2$
M_r = 534.12
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 26.4133 (16) Å
b = 7.6598 (4) Å
c = 18.0332 (11) Å
β = 91.417 (2)°
V = 3647.4 (4) Å^3
Z = 8
F(000) = 2032
D_x = 1.945 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 6743 reflections
θ = 2.7–35.4°
μ = 3.46 mm^{-1}
T = 295 K
Block, colourless
0.26 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and *φ* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.467, T_{max} = 0.545
17839 measured reflections
7647 independent reflections
4855 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 35.9°, θ_{min} = 2.3°
h = −42→42
k = −5→12
l = −29→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.113$
$S = 1.16$
7647 reflections
208 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
$w = 1/[\sigma^2(F_o^2) + (0.0134P)^2 + 27.6528P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.22$ e Å^{-3}
$\Delta\rho_{min} = -1.72$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.198728 (14)	−0.04313 (7)	0.01153 (2)	0.06368 (14)
I2	0.097444 (12)	−0.01689 (5)	0.305807 (16)	0.04538 (10)
O1	−0.25208 (14)	0.6183 (6)	−0.2595 (3)	0.0645 (11)
O2	0.09297 (14)	0.1239 (6)	−0.03377 (17)	0.0567 (10)
H2	0.0683	0.1836	−0.0453	0.085*
N1	0.00453 (14)	0.2516 (5)	−0.0214 (2)	0.0399 (9)
N2	−0.16015 (14)	0.5632 (5)	−0.1763 (2)	0.0425 (9)
C1	0.13595 (16)	0.0208 (6)	0.0746 (2)	0.0369 (9)
C2	0.09350 (17)	0.0948 (6)	0.0387 (2)	0.0373 (9)
C3	0.05152 (15)	0.1370 (6)	0.0821 (2)	0.0335 (9)
C4	0.05340 (16)	0.1049 (6)	0.1581 (2)	0.0361 (9)
H4	0.0257	0.1332	0.1867	0.043*
C5	0.09549 (15)	0.0320 (6)	0.1913 (2)	0.0329 (9)
C6	0.13743 (15)	−0.0108 (6)	0.1495 (2)	0.0337 (9)
H6	0.1660	−0.0601	0.1721	0.040*
C7	0.00713 (17)	0.2167 (6)	0.0481 (3)	0.0395 (10)
H7	−0.0203	0.2434	0.0775	0.047*
C8	−0.03754 (17)	0.3331 (6)	−0.0573 (3)	0.0396 (10)
C9	−0.03566 (18)	0.3557 (7)	−0.1329 (3)	0.0450 (11)
H9	−0.0070	0.3202	−0.1577	0.054*
C10	−0.07575 (19)	0.4305 (7)	−0.1727 (3)	0.0462 (11)
H10	−0.0735	0.4440	−0.2238	0.055*
C11	−0.11929 (17)	0.4858 (6)	−0.1375 (3)	0.0402 (10)
C12	−0.12009 (19)	0.4645 (8)	−0.0609 (3)	0.0505 (13)
H12	−0.1483	0.5023	−0.0355	0.061*
C13	−0.0805 (2)	0.3894 (8)	−0.0215 (3)	0.0520 (13)
H13	−0.0825	0.3762	0.0296	0.062*
C14	−0.1627 (2)	0.5380 (8)	−0.2559 (3)	0.0591 (15)
H14A	−0.1692	0.4159	−0.2668	0.071*
H14B	−0.1305	0.5691	−0.2768	0.071*
C15	−0.2046 (2)	0.6497 (9)	−0.2912 (4)	0.0682 (18)
H15A	−0.1959	0.7720	−0.2852	0.082*
H15B	−0.2069	0.6250	−0.3440	0.082*
C16	−0.2480 (2)	0.6635 (9)	−0.1835 (4)	0.0655 (17)

H16A	−0.2807	0.6489	−0.1611	0.079*
H16B	−0.2385	0.7855	−0.1791	0.079*
C17	−0.20944 (19)	0.5535 (8)	−0.1423 (3)	0.0573 (15)
H17A	−0.2064	0.5932	−0.0913	0.069*
H17B	−0.2208	0.4331	−0.1419	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.04506 (19)	0.1026 (4)	0.04403 (18)	0.0186 (2)	0.01452 (14)	−0.0004 (2)
I2	0.04006 (15)	0.0669 (2)	0.02930 (13)	0.00174 (15)	0.00371 (10)	0.00684 (14)
O1	0.0412 (19)	0.067 (3)	0.084 (3)	−0.0058 (19)	−0.0255 (19)	0.011 (2)
O2	0.059 (2)	0.086 (3)	0.0255 (15)	0.027 (2)	0.0000 (14)	−0.0027 (17)
N1	0.0382 (19)	0.044 (2)	0.0372 (19)	0.0059 (17)	−0.0102 (16)	−0.0042 (17)
N2	0.0365 (19)	0.037 (2)	0.053 (2)	−0.0016 (16)	−0.0128 (17)	0.0076 (18)
C1	0.0314 (19)	0.050 (3)	0.0293 (18)	0.0038 (19)	0.0014 (15)	−0.0053 (19)
C2	0.039 (2)	0.045 (3)	0.0277 (19)	0.000 (2)	−0.0013 (16)	−0.0041 (18)
C3	0.0301 (19)	0.038 (2)	0.0325 (19)	0.0010 (17)	−0.0032 (16)	−0.0035 (17)
C4	0.0287 (19)	0.044 (3)	0.035 (2)	0.0003 (18)	0.0036 (16)	0.0006 (19)
C5	0.0327 (19)	0.041 (2)	0.0249 (16)	−0.0051 (18)	0.0025 (14)	0.0026 (17)
C6	0.0268 (17)	0.043 (2)	0.0316 (18)	0.0002 (17)	−0.0023 (14)	0.0017 (18)
C7	0.031 (2)	0.043 (3)	0.044 (2)	0.0021 (19)	−0.0029 (18)	−0.004 (2)
C8	0.035 (2)	0.039 (2)	0.044 (2)	0.0025 (19)	−0.0085 (18)	−0.001 (2)
C9	0.039 (2)	0.051 (3)	0.046 (3)	0.008 (2)	−0.004 (2)	−0.002 (2)
C10	0.044 (3)	0.052 (3)	0.042 (2)	0.007 (2)	−0.008 (2)	0.000 (2)
C11	0.034 (2)	0.034 (2)	0.052 (3)	−0.0049 (18)	−0.0112 (19)	0.004 (2)
C12	0.037 (2)	0.062 (3)	0.052 (3)	0.010 (2)	−0.002 (2)	0.004 (3)
C13	0.046 (3)	0.069 (4)	0.042 (3)	0.010 (3)	−0.002 (2)	0.006 (3)
C14	0.049 (3)	0.067 (4)	0.060 (3)	0.000 (3)	−0.016 (3)	0.014 (3)
C15	0.056 (3)	0.075 (4)	0.072 (4)	0.003 (3)	−0.024 (3)	0.019 (3)
C16	0.039 (3)	0.071 (4)	0.085 (5)	0.005 (3)	−0.017 (3)	0.012 (4)
C17	0.037 (2)	0.062 (4)	0.073 (4)	0.003 (2)	−0.010 (2)	0.011 (3)

Geometric parameters (Å, º)

I1—C1	2.092 (4)	C8—C9	1.376 (7)
I2—C5	2.097 (4)	C8—C13	1.387 (7)
O1—C15	1.412 (7)	C9—C10	1.389 (6)
O1—C16	1.415 (8)	C9—H9	0.9300
O2—C2	1.325 (5)	C10—C11	1.393 (7)
O2—H2	0.8200	C10—H10	0.9300
N1—C7	1.282 (6)	C11—C12	1.392 (7)
N1—C8	1.417 (6)	C12—C13	1.376 (7)
N2—C11	1.403 (6)	C12—H12	0.9300
N2—C14	1.447 (7)	C13—H13	0.9300
N2—C17	1.455 (7)	C14—C15	1.525 (7)
C1—C6	1.372 (6)	C14—H14A	0.9700
C1—C2	1.401 (6)	C14—H14B	0.9700

C2—C3	1.411 (6)	C15—H15A	0.9700
C3—C4	1.393 (6)	C15—H15B	0.9700
C3—C7	1.445 (6)	C16—C17	1.504 (7)
C4—C5	1.369 (6)	C16—H16A	0.9700
C4—H4	0.9300	C16—H16B	0.9700
C5—C6	1.394 (6)	C17—H17A	0.9700
C6—H6	0.9300	C17—H17B	0.9700
C7—H7	0.9300		

C15—O1—C16	107.7 (4)	C11—C10—H10	119.4
C2—O2—H2	109.5	C12—C11—C10	116.7 (4)
C7—N1—C8	124.1 (4)	C12—C11—N2	120.9 (5)
C11—N2—C14	117.0 (4)	C10—C11—N2	122.3 (5)
C11—N2—C17	117.0 (4)	C13—C12—C11	122.1 (5)
C14—N2—C17	113.0 (4)	C13—C12—H12	118.9
C6—C1—C2	122.0 (4)	C11—C12—H12	118.9
C6—C1—I1	119.4 (3)	C12—C13—C8	120.7 (5)
C2—C1—I1	118.6 (3)	C12—C13—H13	119.7
O2—C2—C1	120.9 (4)	C8—C13—H13	119.7
O2—C2—C3	121.3 (4)	N2—C14—C15	110.8 (5)
C1—C2—C3	117.8 (4)	N2—C14—H14A	109.5
C4—C3—C2	119.8 (4)	C15—C14—H14A	109.5
C4—C3—C7	120.1 (4)	N2—C14—H14B	109.5
C2—C3—C7	120.2 (4)	C15—C14—H14B	109.5
C5—C4—C3	120.8 (4)	H14A—C14—H14B	108.1
C5—C4—H4	119.6	O1—C15—C14	112.2 (5)
C3—C4—H4	119.6	O1—C15—H15A	109.2
C4—C5—C6	120.5 (4)	C14—C15—H15A	109.2
C4—C5—I2	120.2 (3)	O1—C15—H15B	109.2
C6—C5—I2	119.3 (3)	C14—C15—H15B	109.2
C1—C6—C5	119.2 (4)	H15A—C15—H15B	107.9
C1—C6—H6	120.4	O1—C16—C17	112.1 (5)
C5—C6—H6	120.4	O1—C16—H16A	109.2
N1—C7—C3	121.7 (4)	C17—C16—H16A	109.2
N1—C7—H7	119.1	O1—C16—H16B	109.2
C3—C7—H7	119.1	C17—C16—H16B	109.2
C9—C8—C13	118.1 (4)	H16A—C16—H16B	107.9
C9—C8—N1	117.4 (4)	N2—C17—C16	111.4 (5)
C13—C8—N1	124.4 (4)	N2—C17—H17A	109.3
C8—C9—C10	121.3 (5)	C16—C17—H17A	109.3
C8—C9—H9	119.4	N2—C17—H17B	109.3
C10—C9—H9	119.4	C16—C17—H17B	109.3
C9—C10—C11	121.1 (5)	H17A—C17—H17B	108.0
C9—C10—H10	119.4		

C6—C1—C2—O2	−179.9 (5)	N1—C8—C9—C10	178.4 (5)
I1—C1—C2—O2	0.0 (7)	C8—C9—C10—C11	0.1 (8)
C6—C1—C2—C3	0.1 (7)	C9—C10—C11—C12	0.9 (8)

I1—C1—C2—C3	180.0 (3)	C9—C10—C11—N2	179.4 (5)
O2—C2—C3—C4	−179.9 (5)	C14—N2—C11—C12	−163.6 (5)
C1—C2—C3—C4	0.1 (7)	C17—N2—C11—C12	−24.8 (7)
O2—C2—C3—C7	−1.2 (7)	C14—N2—C11—C10	17.9 (7)
C1—C2—C3—C7	178.8 (4)	C17—N2—C11—C10	156.7 (5)
C2—C3—C4—C5	−0.2 (7)	C10—C11—C12—C13	−1.3 (8)
C7—C3—C4—C5	−178.9 (4)	N2—C11—C12—C13	−179.9 (5)
C3—C4—C5—C6	0.2 (7)	C11—C12—C13—C8	0.7 (9)
C3—C4—C5—I2	−179.6 (3)	C9—C8—C13—C12	0.4 (8)
C2—C1—C6—C5	−0.1 (7)	N1—C8—C13—C12	−178.8 (5)
I1—C1—C6—C5	180.0 (3)	C11—N2—C14—C15	−172.1 (5)
C4—C5—C6—C1	−0.1 (7)	C17—N2—C14—C15	47.5 (6)
I2—C5—C6—C1	179.8 (3)	C16—O1—C15—C14	61.6 (7)
C8—N1—C7—C3	−178.5 (4)	N2—C14—C15—O1	−55.3 (7)
C4—C3—C7—N1	178.5 (5)	C15—O1—C16—C17	−61.9 (6)
C2—C3—C7—N1	−0.2 (7)	C11—N2—C17—C16	171.5 (5)
C7—N1—C8—C9	−177.4 (5)	C14—N2—C17—C16	−48.1 (7)
C7—N1—C8—C13	1.7 (8)	O1—C16—C17—N2	55.7 (7)
C13—C8—C9—C10	−0.8 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1	0.82	1.82	2.548 (5)	146
C6—H6···O1^{i}	0.93	2.50	3.413 (5)	166

Symmetry code: (i) *x*+1/2, −*y*+1/2, *z*+1/2.