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2,4-Dibromo-6-(cyclopropyliminomethyl)phenol

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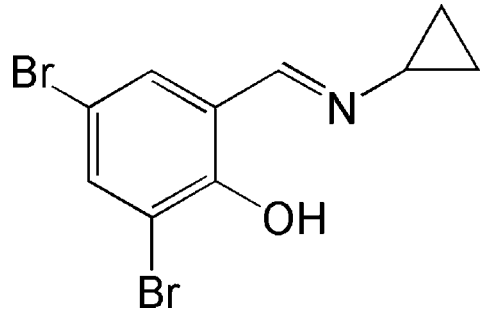
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.045; wR factor = 0.105; data-to-parameter ratio = 18.9.

The asymmetric unit of the title compound, $C_{10}H_9Br_2NO$, consists of two molecules. In both molecules, the benzene and cyclopropyl rings are nearly perpendicular, with dihedral angles of 85.8 (4) and 75.5 (4)°. In the crystal structure, there are no obviously short intermolecular contacts. Each molecule has an intramolecular O—H···N hydrogen bond.

Related literature

For related structures see Yang (2006*a*,*b*,*c*,*d*,*e*, 2007); Yang & Guo (2006); Zhao (2005); You & Chi (2006). For related literature, see: Allen *et al.* (1987); Bernardo *et al.* (1996); Musie *et al.* (2001); Paul *et al.* (2002).



Experimental

Crystal data

$C_{10}H_9Br_2NO$
M_r = 319.00
Triclinic, $P\overline{1}$
a = 9.1840 (18) Å
b = 11.495 (2) Å
c = 12.265 (3) Å
α = 70.85 (3)°
β = 68.62 (3)°
γ = 69.69 (3)°
V = 1100.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.33 mm^{-1}
T = 298 (2) K
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.157, T_{max} = 0.322
(expected range = 0.113–0.231)
9324 measured reflections
4830 independent reflections
2945 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.105
S = 0.95
4830 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N2	0.82	1.90	2.607 (5)	143
O1—H1···N1	0.82	1.87	2.597 (5)	147

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: OM2147).

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supplementary materials

Acta Cryst. (2007). E**63**, o3737 [**doi:10.1107/S1600536807038494**]

2,4-Dibromo-6-(cyclopropyliminomethyl)phenol

D.-S. Yang

Comment

Schiff base compounds have been of great interest for a long time. These compounds play an important role in the development of coordination chemistry (Musie *et al.*, 2001; Bernardo *et al.*, 1996; Paul *et al.*, 2002). Recently, we have reported a few Schiff base compounds (Yang, 2006*a*,b,c,d,e, 2007; Yang & Guo, 2006). As a further investigation of this work, the crystal structure of the title compound is reported here.

The asymmetric unit of the title compound consists of two molecules (Fig. 1). In both molecules, the benzene ring and the cyclopropyl ring are nearly perpendicular, with the dihedral angles of 85.8 (4) and 75.5 (4)°, respectively. All the bond lengths in the molecules are within normal ranges (Allen *et al.*, 1987), and comparable to those of the similar compounds (Zhao, 2005, You & Chi, 2006). The C7═N1 and C17═N2 bond lengths of 1.272 (5) and 1.276 (5) Å conform to the values for double bonds. In the crystal structure, there are no obviously short contacts among the molecules.

Experimental

3,5-Dibromosalicylaldehyde (0.1 mmol, 18.0 mg) and cyclopropylamine (0.1 mmol, 5.7 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature to give a clear yellow solution. Crystals of the title compound were formed by gradual evaporation of the solvent over a period of about one week at room temperature.

Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with O—H distances of 0.82 Å, C—H distances of 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Figures

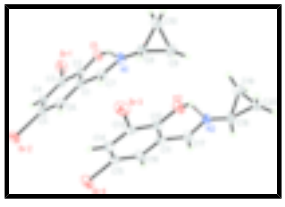


Fig. 1. The structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

2,4-Dibromo-6-(cyclopropyliminomethyl)phenol

Crystal data

$C_{10}H_9Br_2NO$	$Z = 4$
$M_r = 319.00$	$F_{000} = 616$

Triclinic, $P\bar{1}$	D_x = 1.926 Mg m^{-3}
a = 9.1840 (18) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 11.495 (2) Å	Cell parameters from 2313 reflections
c = 12.265 (3) Å	θ = 2.4–25.1º
α = 70.85 (3)º	μ = 7.33 mm^{-1}
β = 68.62 (3)º	T = 298 (2) K
γ = 69.69 (3)º	Block, yellow
V = 1100.2 (4) Å^3	0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer	4830 independent reflections
Radiation source: fine-focus sealed tube	2945 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.157, T_{max} = 0.322	k = −14→14
9324 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.95	$(\Delta/\sigma)_{max} < 0.001$
4830 reflections	$\Delta\rho_{max}$ = 0.64 e Å^{-3}
255 parameters	$\Delta\rho_{min}$ = −0.69 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	−0.11261 (8)	−0.17137 (5)	0.31199 (6)	0.0654 (2)
Br2	0.54050 (7)	−0.29887 (5)	0.31061 (5)	0.05466 (18)
Br3	0.48615 (7)	0.32486 (6)	0.37844 (5)	0.0631 (2)
Br4	0.67363 (7)	0.01999 (5)	0.04642 (5)	0.05876 (19)
O1	−0.1149 (4)	0.0760 (3)	0.3466 (3)	0.0472 (8)
H1	−0.1128	0.1446	0.3518	0.071*
O2	0.3037 (4)	0.5125 (3)	0.2034 (3)	0.0462 (8)
H2	0.2358	0.5531	0.1669	0.069*
N1	0.0071 (5)	0.2383 (3)	0.3665 (3)	0.0427 (10)
N2	0.1932 (4)	0.5883 (3)	0.0169 (3)	0.0384 (9)
C1	0.1612 (6)	0.0265 (4)	0.3465 (4)	0.0363 (11)
C2	0.0329 (6)	−0.0049 (4)	0.3375 (4)	0.0361 (11)
C3	0.0627 (6)	−0.1257 (4)	0.3186 (4)	0.0400 (11)
C4	0.2121 (6)	−0.2115 (4)	0.3086 (4)	0.0418 (12)
H4	0.2293	−0.2909	0.2950	0.050*
C5	0.3354 (6)	−0.1783 (4)	0.3188 (4)	0.0407 (11)
C6	0.3111 (6)	−0.0607 (4)	0.3378 (4)	0.0405 (11)
H6	0.3958	−0.0397	0.3449	0.049*
C7	0.1393 (6)	0.1521 (4)	0.3654 (4)	0.0411 (11)
H7	0.2241	0.1690	0.3767	0.049*
C8	−0.0023 (6)	0.3593 (4)	0.3822 (5)	0.0461 (13)
H8	0.0894	0.3654	0.4011	0.055*
C9	−0.0850 (7)	0.4753 (5)	0.3070 (5)	0.0587 (15)
H9A	−0.0430	0.5497	0.2794	0.070*
H9B	−0.1274	0.4635	0.2507	0.070*
C10	−0.1668 (7)	0.4377 (5)	0.4370 (5)	0.0597 (15)
H10A	−0.2586	0.4026	0.4600	0.072*
H10B	−0.1741	0.4890	0.4887	0.072*
C11	0.3820 (5)	0.3853 (4)	0.0594 (4)	0.0347 (10)
C12	0.3856 (5)	0.4019 (4)	0.1673 (4)	0.0340 (10)
C13	0.4791 (5)	0.3044 (4)	0.2334 (4)	0.0372 (11)
C14	0.5632 (5)	0.1906 (4)	0.1997 (4)	0.0384 (11)
H14	0.6235	0.1251	0.2467	0.046*
C15	0.5562 (5)	0.1755 (4)	0.0950 (4)	0.0380 (11)
C16	0.4685 (5)	0.2713 (4)	0.0247 (4)	0.0401 (12)
H16	0.4669	0.2599	−0.0465	0.048*
C17	0.2896 (5)	0.4881 (4)	−0.0175 (4)	0.0391 (11)
H17	0.3018	0.4798	−0.0935	0.047*
C18	0.1096 (6)	0.6847 (4)	−0.0628 (4)	0.0445 (12)
H18	0.1489	0.6790	−0.1471	0.053*
C19	−0.0688 (6)	0.7366 (5)	−0.0140 (5)	0.0579 (15)
H19A	−0.1357	0.7597	−0.0673	0.069*
H19B	−0.1192	0.7019	0.0698	0.069*
C20	0.0415 (6)	0.8155 (4)	−0.0400 (5)	0.0476 (13)
H20A	0.0586	0.8294	0.0277	0.057*

H20B	0.0422	0.8872	−0.1093	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0728 (4)	0.0560 (4)	0.0896 (5)	−0.0173 (3)	−0.0424 (4)	−0.0221 (3)
Br2	0.0543 (4)	0.0474 (3)	0.0566 (4)	0.0070 (2)	−0.0191 (3)	−0.0225 (3)
Br3	0.0665 (4)	0.0767 (4)	0.0512 (4)	0.0029 (3)	−0.0293 (3)	−0.0300 (3)
Br4	0.0586 (4)	0.0438 (3)	0.0791 (4)	0.0062 (2)	−0.0294 (3)	−0.0304 (3)
O1	0.050 (2)	0.0368 (19)	0.057 (2)	−0.0050 (16)	−0.0227 (18)	−0.0119 (17)
O2	0.048 (2)	0.043 (2)	0.051 (2)	−0.0001 (15)	−0.0168 (17)	−0.0238 (17)
N1	0.049 (3)	0.030 (2)	0.047 (3)	−0.0089 (19)	−0.013 (2)	−0.0089 (18)
N2	0.035 (2)	0.036 (2)	0.043 (2)	−0.0059 (18)	−0.0137 (19)	−0.0076 (18)
C1	0.044 (3)	0.029 (2)	0.036 (3)	−0.010 (2)	−0.010 (2)	−0.007 (2)
C2	0.043 (3)	0.029 (2)	0.029 (3)	−0.003 (2)	−0.010 (2)	−0.0046 (19)
C3	0.058 (3)	0.036 (3)	0.035 (3)	−0.016 (2)	−0.023 (2)	−0.004 (2)
C4	0.055 (3)	0.031 (3)	0.040 (3)	−0.001 (2)	−0.021 (2)	−0.012 (2)
C5	0.045 (3)	0.033 (3)	0.040 (3)	0.000 (2)	−0.014 (2)	−0.011 (2)
C6	0.039 (3)	0.045 (3)	0.038 (3)	−0.013 (2)	−0.008 (2)	−0.010 (2)
C7	0.041 (3)	0.033 (3)	0.044 (3)	−0.008 (2)	−0.008 (2)	−0.009 (2)
C8	0.047 (3)	0.027 (2)	0.066 (3)	−0.005 (2)	−0.019 (3)	−0.015 (2)
C9	0.077 (4)	0.037 (3)	0.062 (4)	−0.021 (3)	−0.019 (3)	−0.005 (3)
C10	0.062 (4)	0.040 (3)	0.066 (4)	−0.003 (3)	−0.008 (3)	−0.019 (3)
C11	0.028 (3)	0.039 (3)	0.038 (3)	−0.007 (2)	−0.008 (2)	−0.014 (2)
C12	0.029 (3)	0.036 (3)	0.040 (3)	−0.008 (2)	−0.008 (2)	−0.014 (2)
C13	0.034 (3)	0.048 (3)	0.034 (3)	−0.014 (2)	−0.008 (2)	−0.013 (2)
C14	0.028 (3)	0.041 (3)	0.044 (3)	−0.009 (2)	−0.012 (2)	−0.005 (2)
C15	0.031 (3)	0.036 (3)	0.047 (3)	−0.007 (2)	−0.007 (2)	−0.015 (2)
C16	0.037 (3)	0.041 (3)	0.047 (3)	−0.004 (2)	−0.015 (2)	−0.019 (2)
C17	0.040 (3)	0.041 (3)	0.040 (3)	−0.009 (2)	−0.017 (2)	−0.010 (2)
C18	0.045 (3)	0.039 (3)	0.043 (3)	0.001 (2)	−0.019 (2)	−0.008 (2)
C19	0.038 (3)	0.060 (4)	0.072 (4)	−0.007 (3)	−0.025 (3)	−0.006 (3)
C20	0.045 (3)	0.040 (3)	0.051 (3)	−0.005 (2)	−0.015 (3)	−0.006 (2)

Geometric parameters (Å, °)

Br1—C3	1.894 (5)	C8—H8	0.9800
Br2—C5	1.903 (4)	C9—C10	1.481 (7)
Br3—C13	1.895 (4)	C9—H9A	0.9700
Br4—C15	1.899 (4)	C9—H9B	0.9700
O1—C2	1.342 (5)	C10—H10A	0.9700
O1—H1	0.8200	C10—H10B	0.9700
O2—C12	1.356 (5)	C11—C16	1.389 (6)
O2—H2	0.8200	C11—C12	1.410 (6)
N1—C7	1.272 (5)	C11—C17	1.471 (6)
N1—C8	1.436 (5)	C12—C13	1.377 (6)
N2—C17	1.276 (5)	C13—C14	1.379 (6)
N2—C18	1.421 (5)	C14—C15	1.376 (6)
C1—C6	1.384 (6)	C14—H14	0.9300

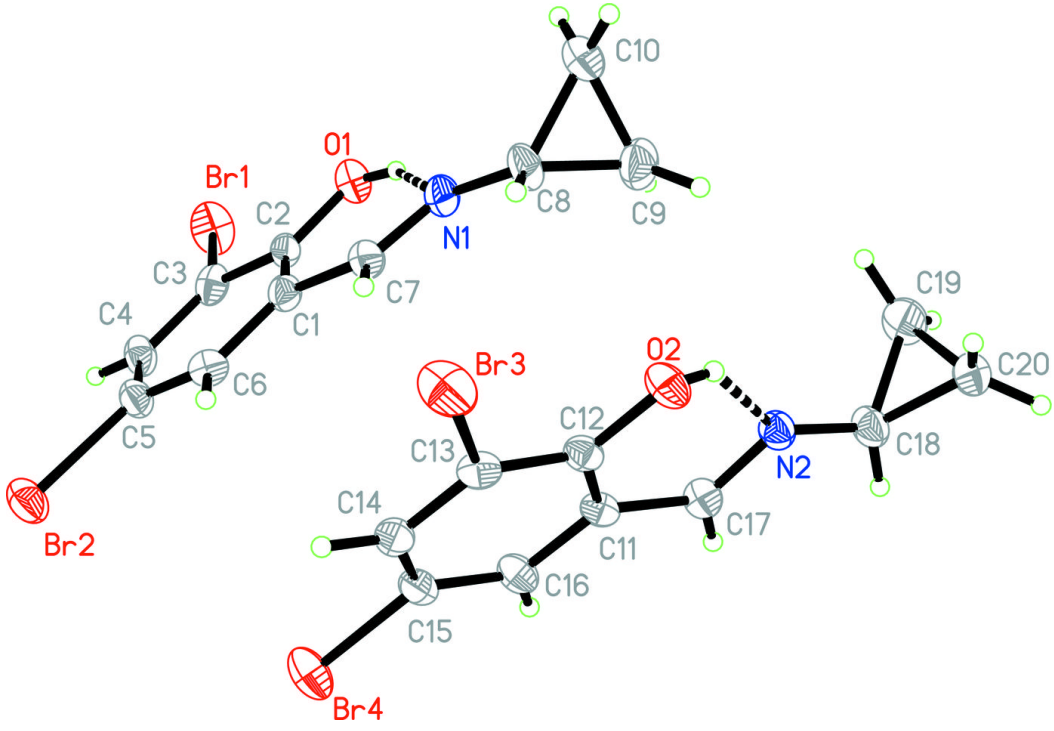
C1—C2	1.396 (6)	C15—C16	1.368 (6)
C1—C7	1.470 (6)	C16—H16	0.9300
C2—C3	1.398 (6)	C17—H17	0.9300
C3—C4	1.375 (6)	C18—C20	1.492 (6)
C4—C5	1.371 (6)	C18—C19	1.496 (7)
C4—H4	0.9300	C18—H18	0.9800
C5—C6	1.374 (6)	C19—C20	1.470 (7)
C6—H6	0.9300	C19—H19A	0.9700
C7—H7	0.9300	C19—H19B	0.9700
C8—C9	1.485 (6)	C20—H20A	0.9700
C8—C10	1.503 (6)	C20—H20B	0.9700
C2—O1—H1	109.5	C8—C10—H10B	117.8
C12—O2—H2	109.5	H10A—C10—H10B	114.9
C7—N1—C8	117.8 (4)	C16—C11—C12	119.6 (4)
C17—N2—C18	118.9 (4)	C16—C11—C17	119.6 (4)
C6—C1—C2	120.1 (4)	C12—C11—C17	120.7 (4)
C6—C1—C7	119.2 (4)	O2—C12—C13	120.5 (4)
C2—C1—C7	120.7 (4)	O2—C12—C11	121.2 (4)
O1—C2—C1	122.3 (4)	C13—C12—C11	118.3 (4)
O1—C2—C3	120.1 (4)	C12—C13—C14	122.0 (4)
C1—C2—C3	117.6 (4)	C12—C13—Br3	119.0 (3)
C4—C3—C2	122.1 (4)	C14—C13—Br3	118.9 (3)
C4—C3—Br1	120.0 (3)	C15—C14—C13	118.8 (4)
C2—C3—Br1	117.9 (4)	C15—C14—H14	120.6
C5—C4—C3	118.9 (4)	C13—C14—H14	120.6
C5—C4—H4	120.6	C16—C15—C14	121.2 (4)
C3—C4—H4	120.6	C16—C15—Br4	119.6 (3)
C4—C5—C6	120.8 (4)	C14—C15—Br4	119.2 (3)
C4—C5—Br2	119.1 (3)	C15—C16—C11	120.1 (4)
C6—C5—Br2	120.0 (4)	C15—C16—H16	120.0
C5—C6—C1	120.4 (4)	C11—C16—H16	120.0
C5—C6—H6	119.8	N2—C17—C11	122.0 (4)
C1—C6—H6	119.8	N2—C17—H17	119.0
N1—C7—C1	121.5 (5)	C11—C17—H17	119.0
N1—C7—H7	119.2	N2—C18—C20	118.0 (4)
C1—C7—H7	119.2	N2—C18—C19	117.6 (4)
N1—C8—C9	117.2 (4)	C20—C18—C19	59.0 (3)
N1—C8—C10	117.4 (4)	N2—C18—H18	116.6
C9—C8—C10	59.4 (3)	C20—C18—H18	116.6
N1—C8—H8	116.8	C19—C18—H18	116.6
C9—C8—H8	116.8	C20—C19—C18	60.4 (3)
C10—C8—H8	116.8	C20—C19—H19A	117.7
C10—C9—C8	60.9 (3)	C18—C19—H19A	117.7
C10—C9—H9A	117.7	C20—C19—H19B	117.7
C8—C9—H9A	117.7	C18—C19—H19B	117.7
C10—C9—H9B	117.7	H19A—C19—H19B	114.9
C8—C9—H9B	117.7	C19—C20—C18	60.7 (3)
H9A—C9—H9B	114.8	C19—C20—H20A	117.7
C9—C10—C8	59.7 (3)	C18—C20—H20A	117.7

C9—C10—H10A	117.8	C19—C20—H20B	117.7
C8—C10—H10A	117.8	C18—C20—H20B	117.7
C9—C10—H10B	117.8	H20A—C20—H20B	114.8

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N2	0.82	1.90	2.607 (5)	143
O1—H1···N1	0.82	1.87	2.597 (5)	147

Fig. 1


C10
O1
Br1
C2
C8
C9
N1
C3
C7
C19
C4
C1
Br3
O2
C20
C6
C12
C5
C13
N2
C18
C14
C17
Br2
C11
C16
C15
Br4