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rac-(*Z*)-2-(2,4-Dichlorobenzylidene)-1-azabicyclo[2.2.2]octan-3-ol

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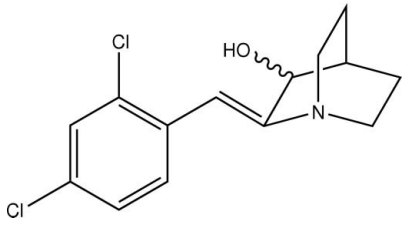
Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.034; wR factor = 0.089; data-to-parameter ratio = 16.4.

The racemic form of the title compound, $C_{14}H_{15}Cl_2NO$, was prepared by the base-catalyzed reaction of 2,4-dichlorobenzaldehyde with 1-azabicyclo[2.2.2]octan-3-one and subsequent reduction to the corresponding secondary alcohol. In the molecule, the olefinic bond connecting the 2,4-dichlorophenyl ring and 1-azabicyclo[2.2.2]octan-3-ol group has *Z* geometry. The C=C—CH=C torsion angle [45.3 (3)°] indicates deviation of the 2,4-dichlorophenyl ring from the plane of the double bond connected to the azabicyclic ring. The hydroxyl group is disordered over two sites, the ratio of occupancies being approximately 0.67:0.33. The crystal structure contains intermolecular O—H···N hydrogen bonds.

Related literature

For related literature, see: Sekhar *et al.* (2007); Sonar *et al.* (2004); Wilson (1992).



Experimental

Crystal data

$C_{14}H_{15}Cl_2NO$
M_r = 284.17
Triclinic, $P\overline{1}$
a = 6.1374 (1) Å
b = 10.3379 (2) Å
c = 10.6340 (2) Å
α = 107.269 (1)°
β = 98.391 (1)°
γ = 96.098 (1)°
V = 629.36 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.50 mm^{-1}
T = 90.0 (2) K
0.40 × 0.30 × 0.25 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.825, T_{max} = 0.885
5704 measured reflections
2873 independent reflections
2459 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
S = 1.07
2873 reflections
175 parameters
21 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O16—H16···N9^{i}	0.84	2.05	2.872 (2)	166

Symmetry code: (i) $x-1, y, z$.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELX97* and local procedures.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2483).

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supplementary materials

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rac-(*Z*)-2-(2,4-Dichlorobenzylidene)-1-azabicyclo[2.2.2]octan-3-ol

V. N. Sonar, S. Parkin and P. A. Crooks

Comment

Radio-sensitizers are drugs that make cancer cells more sensitive to radiation therapy. Radiation therapy prevents cancer cells from growing and dividing. Radiation therapy, however, can also damage normal cells. Consequently, researchers are looking for substances that can either make a tumor more sensitive to radiation without affecting healthy tissues, or that can shield normal cells from radiation. Recently, we have reported (Sekhar *et al.*, 2007) on the radio-sensitizing activity of *N*-arylsubstituted rac-(*Z*)-2-(1*H*-indol-3-ylmethylene)-1-azabicyclo[2.2.2]octan −3-ols. In addition to these indole analogues, we also synthesized 1-azabicyclo[2.2.2]octan-3-ols linked to non-indolic systems to compare their radio-sensitizing activities with those of the indole analogs.

In order to confirm the double-bond geometry, and to determine the molecular conformation in the crystal structure, the X-ray analysis of the title compound has been carried out. The molecular structure and atom-numbering scheme for the title molecule is shown in Fig. 1. The title molecule comprises a 1-azabicyclo[2.2.2]octan-3-ol moiety and a 2,4-dichlorophenyl group linked *via* a C7═C8 bond that has the *Z* geometry. The bond angles around the C7 and C8 atoms deviate from the ideal value [120°]; the angles for N9—C8—C13, and C7=C8—C1 [114.16 (14), and 128.31 (15)°, respectively] are distorted, as a consequence of the strain induced by the double bond linkage at C7═C8. These deviations contribute to the release of the intramolecular nonbonded interactions. The C2═C1—C7═C8 torsion angle [45.3 (3)°] indicates a deviation of the 2,4-dichlorophenyl ring from the plane of the double bond connected to the azabicyclic ring. Also, the C1—C7 bond length [1.472 (2) Å], in comparison with the standard value for a C_{ar}—C_{sp^2} single bond [1.470 (15) Å; Wilson, 1992], suggests a lack of conjugation to the 2,4-dichlorophenyl ring.

Experimental

The title compound was prepared according to the previously reported procedure of Sonar *et al.* (2004). Crystallization from ethyl acetate afforded colorless crystals. ^{1}H NMR ($CDCl_3$, p.p.m.): δ 1.42–1.61 (m, 2H), 1.69–1.78 (m, 1H), 1.79–1.99 (m, 2H), 2.07 (p, 1H), 2.68–2.78 (m, 1H), 2.91–3.01 (m, 3H), 4.34 (p, 1H), 6.60 (d, 1H), 7.17 (dt, 1H), 7.35 (d, 1H), 8.21 (d, 1H). ^{13}C NMR ($CDCl_3$, p.p.m.): δ 19.17, 25.28, 31.05, 47.36, 48.38, 71.35, 117.51, 126.88, 128.90, 132.13, 132.30, 132.83, 133.82, 155.06.

Refinement

H atoms were found in difference Fourier maps and subsequently placed in idealized positions with constrained C—H distances of 1.00 Å (R_3CH), 0.99 Å (R_2CH_2), 0.95 Å ($C_{Ar}H$) and 0.84 Å (OH). U_{iso}(H) values were set to either 1.2U_{eq}(C) or 1.5U_{eq}(O). The hydroxyl group is disordered over two sites with occupancy factors 0.67:0.33, and the hydroxyl hydrogen is also disordered. The major component was placed the position of maximum electron density as calculated in a torus beyond

the oxygen atom labelled O16, while the minor component was placed in the most reasonable hydrogen bonding position, as dictated by the *SHELXL* (Sheldrick, 1997) commands "HFIX 147" and "HFIX 87" respectively.

Figures

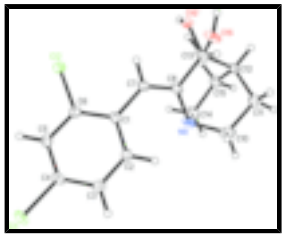

Fig. 1. A view of the title molecule, with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The hydroxyl group is disordered.

rac-(*Z*)-2-(2,4-Dichlorobenzylidene)-1-azabicyclo[2.2.2]octan-3-ol

Crystal data

$C_{14}H_{15}Cl_2NO$	$Z = 2$
$M_r = 284.17$	$F_{000} = 296$
Triclinic, $P\overline{1}$	$D_x = 1.500$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.1374$ (1) Å	Cell parameters from 2861 reflections
$b = 10.3379$ (2) Å	$\theta = 1.0$–27.5°
$c = 10.6340$ (2) Å	$\mu = 0.50$ mm^{-1}
$\alpha = 107.269$ (1)°	$T = 90.0$ (2) K
$\beta = 98.391$ (1)°	Block, colourless
$\gamma = 96.098$ (1)°	0.40 × 0.30 × 0.25 mm
$V = 629.36$ (2) Å^3	

Data collection

Nonius KappaCCD area-detector diffractometer	2873 independent reflections
Radiation source: fine-focus sealed tube	2459 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
Detector resolution: 18 pixels mm^{-1}	$\theta_{max} = 27.5^\circ$
$T = 90.0(2)$ K	$\theta_{min} = 2.0^\circ$
ω scans at fixed $\chi = 55°$	$h = -7 \rightarrow 7$
Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)	$k = -13 \rightarrow 13$
$T_{min} = 0.825$, $T_{max} = 0.885$	$l = -13 \rightarrow 13$
5704 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 0.4377P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
2873 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
175 parameters	$\Delta\rho_{min} = -0.59$ e Å^{-3}
21 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\sigma(F^2)$ 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}	Occ. (<1)
Cl1	0.98623 (7)	0.11120 (4)	0.35241 (4)	0.02142 (12)	
Cl2	0.21149 (7)	0.13519 (4)	0.05932 (4)	0.01986 (12)	
C1	0.4485 (3)	0.35709 (16)	0.25998 (16)	0.0140 (3)	
C2	0.6331 (3)	0.41588 (17)	0.36374 (17)	0.0172 (3)	
H2	0.6457	0.5096	0.4156	0.021*	
C3	0.7983 (3)	0.34190 (17)	0.39344 (17)	0.0178 (3)	
H3	0.9209	0.3838	0.4651	0.021*	
C4	0.7811 (3)	0.20619 (16)	0.31682 (16)	0.0152 (3)	
C5	0.6030 (3)	0.14248 (16)	0.21268 (15)	0.0154 (3)	
H5	0.5933	0.0493	0.1601	0.018*	
C6	0.4387 (3)	0.21898 (16)	0.18738 (15)	0.0142 (3)	
C7	0.2664 (3)	0.43339 (16)	0.23489 (16)	0.0162 (3)	
H7	0.1195	0.3850	0.2196	0.019*	
C8	0.2812 (3)	0.56122 (18)	0.2309 (2)	0.0234 (4)	
N9	0.4903 (2)	0.64743 (15)	0.24100 (18)	0.0263 (4)	
C10	0.5113 (3)	0.77456 (19)	0.3572 (2)	0.0276 (4)	
H10A	0.6543	0.8340	0.3665	0.033*	
H10B	0.5135	0.7497	0.4403	0.033*	
C11	0.3171 (3)	0.85452 (18)	0.33952 (17)	0.0210 (4)	
H11A	0.2408	0.8685	0.4173	0.025*	
H11B	0.3751	0.9457	0.3346	0.025*	

C12	0.1525 (3)	0.77320 (16)	0.21067 (17)	0.0173 (3)	
H12	0.0217	0.8215	0.1994	0.021*	
C13	0.0756 (3)	0.63001 (19)	0.2150 (3)	0.0355 (5)	
H13	−0.0158	0.5773	0.1247	0.043*	0.666 (4)
H13'	0.0486	0.6543	0.3091	0.043*	0.334 (4)
C14	0.4787 (3)	0.68899 (19)	0.1179 (2)	0.0284 (4)	
H14A	0.4768	0.6072	0.0400	0.034*	
H14B	0.6142	0.7549	0.1273	0.034*	
C15	0.2710 (3)	0.75526 (19)	0.09092 (18)	0.0236 (4)	
H15A	0.3155	0.8455	0.0797	0.028*	
H15B	0.1698	0.6959	0.0078	0.028*	
O16	−0.0490 (3)	0.6203 (2)	0.30373 (19)	0.0229 (5)	0.666 (4)
H16	−0.1830	0.6192	0.2718	0.034*	0.666 (4)
O16'	−0.0997 (5)	0.5521 (3)	0.1570 (4)	0.0174 (10)	0.334 (4)
H16'	−0.1107	0.5351	0.0738	0.026*	0.334 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0206 (2)	0.0230 (2)	0.0238 (2)	0.01253 (16)	0.00340 (16)	0.00927 (17)
Cl2	0.0184 (2)	0.0187 (2)	0.0192 (2)	0.00315 (15)	−0.00177 (15)	0.00352 (15)
C1	0.0128 (7)	0.0147 (7)	0.0177 (7)	0.0034 (6)	0.0062 (6)	0.0080 (6)
C2	0.0161 (8)	0.0126 (8)	0.0215 (8)	0.0025 (6)	0.0038 (6)	0.0033 (6)
C3	0.0148 (8)	0.0177 (8)	0.0196 (8)	0.0019 (6)	0.0006 (6)	0.0055 (6)
C4	0.0138 (7)	0.0180 (8)	0.0182 (7)	0.0077 (6)	0.0051 (6)	0.0095 (6)
C5	0.0183 (8)	0.0137 (8)	0.0156 (7)	0.0037 (6)	0.0059 (6)	0.0050 (6)
C6	0.0138 (7)	0.0155 (8)	0.0140 (7)	0.0012 (6)	0.0030 (6)	0.0057 (6)
C7	0.0107 (7)	0.0156 (8)	0.0230 (8)	0.0025 (6)	0.0043 (6)	0.0066 (6)
C8	0.0100 (8)	0.0181 (9)	0.0450 (11)	0.0036 (6)	0.0056 (7)	0.0134 (8)
N9	0.0095 (7)	0.0184 (7)	0.0562 (11)	0.0027 (6)	0.0050 (7)	0.0200 (7)
C10	0.0166 (8)	0.0241 (9)	0.0429 (11)	−0.0015 (7)	−0.0058 (8)	0.0186 (8)
C11	0.0168 (8)	0.0254 (9)	0.0209 (8)	0.0047 (7)	0.0031 (6)	0.0073 (7)
C12	0.0117 (7)	0.0133 (8)	0.0268 (9)	0.0041 (6)	0.0011 (6)	0.0067 (6)
C13	0.0113 (8)	0.0195 (9)	0.0826 (17)	0.0043 (7)	0.0093 (9)	0.0255 (10)
C14	0.0220 (9)	0.0206 (9)	0.0488 (12)	0.0087 (7)	0.0158 (8)	0.0139 (8)
C15	0.0197 (9)	0.0247 (9)	0.0227 (9)	0.0063 (7)	0.0012 (7)	0.0022 (7)
O16	0.0126 (9)	0.0333 (12)	0.0320 (11)	0.0090 (8)	0.0086 (8)	0.0202 (9)
O16'	0.0111 (17)	0.0147 (18)	0.0239 (19)	0.0009 (13)	−0.0002 (13)	0.0043 (14)

Geometric parameters (Å, °)

Cl1—C4	1.7425 (16)	C10—H10A	0.9900
Cl2—C6	1.7430 (16)	C10—H10B	0.9900
C1—C6	1.397 (2)	C11—C12	1.529 (2)
C1—C2	1.401 (2)	C11—H11A	0.9900
C1—C7	1.472 (2)	C11—H11B	0.9900
C2—C3	1.388 (2)	C12—C13	1.521 (2)
C2—H2	0.9500	C12—C15	1.531 (2)
C3—C4	1.381 (2)	C12—H12	1.0000

C3—H3	0.9500	C13—O16'	1.231 (4)
C4—C5	1.384 (2)	C13—O16	1.318 (3)
C5—C6	1.390 (2)	C13—H13	1.0000
C5—H5	0.9500	C13—H13'	1.0000
C7—C8	1.329 (2)	C14—C15	1.540 (2)
C7—H7	0.9500	C14—H14A	0.9900
C8—N9	1.453 (2)	C14—H14B	0.9900
C8—C13	1.525 (2)	C15—H15A	0.9900
N9—C14	1.489 (3)	C15—H15B	0.9900
N9—C10	1.491 (3)	O16—H16	0.8400
C10—C11	1.542 (2)	O16'—H16'	0.8400
C6—C1—C2	116.32 (14)	C12—C11—H11B	109.9
C6—C1—C7	121.62 (14)	C10—C11—H11B	109.9
C2—C1—C7	121.92 (14)	H11A—C11—H11B	108.3
C3—C2—C1	122.23 (15)	C13—C12—C11	109.58 (15)
C3—C2—H2	118.9	C13—C12—C15	106.75 (15)
C1—C2—H2	118.9	C11—C12—C15	109.35 (13)
C4—C3—C2	118.79 (15)	C13—C12—H12	110.4
C4—C3—H3	120.6	C11—C12—H12	110.4
C2—C3—H3	120.6	C15—C12—H12	110.4
C3—C4—C5	121.66 (14)	O16'—C13—O16	70.8 (2)
C3—C4—Cl1	119.60 (12)	O16'—C13—C12	128.5 (2)
C5—C4—Cl1	118.73 (12)	O16—C13—C12	117.11 (19)
C4—C5—C6	117.97 (14)	O16'—C13—C8	115.7 (2)
C4—C5—H5	121.0	O16—C13—C8	111.26 (18)
C6—C5—H5	121.0	C12—C13—C8	107.96 (14)
C5—C6—C1	123.01 (14)	O16—C13—H13	106.6
C5—C6—Cl2	117.20 (12)	C12—C13—H13	106.6
C1—C6—Cl2	119.79 (12)	C8—C13—H13	106.6
C8—C7—C1	128.31 (15)	O16'—C13—H13'	99.3
C8—C7—H7	115.8	C12—C13—H13'	99.3
C1—C7—H7	115.8	C8—C13—H13'	99.3
C7—C8—N9	123.90 (15)	H13—C13—H13'	134.9
C7—C8—C13	121.94 (15)	N9—C14—C15	112.54 (15)
N9—C8—C13	114.16 (14)	N9—C14—H14A	109.1
C8—N9—C14	108.26 (15)	C15—C14—H14A	109.1
C8—N9—C10	108.20 (15)	N9—C14—H14B	109.1
C14—N9—C10	107.50 (14)	C15—C14—H14B	109.1
N9—C10—C11	111.53 (14)	H14A—C14—H14B	107.8
N9—C10—H10A	109.3	C12—C15—C14	108.05 (15)
C11—C10—H10A	109.3	C12—C15—H15A	110.1
N9—C10—H10B	109.3	C14—C15—H15A	110.1
C11—C10—H10B	109.3	C12—C15—H15B	110.1
H10A—C10—H10B	108.0	C14—C15—H15B	110.1
C12—C11—C10	109.14 (14)	H15A—C15—H15B	108.4
C12—C11—H11A	109.9	C13—O16—H16	109.5
C10—C11—H11A	109.9	C13—O16'—H16'	109.5
C6—C1—C2—C3	0.1 (2)	C14—N9—C10—C11	56.80 (18)

C7—C1—C2—C3	175.79 (15)	N9—C10—C11—C12	3.6 (2)
C1—C2—C3—C4	0.9 (2)	C10—C11—C12—C13	55.83 (19)
C2—C3—C4—C5	−0.6 (2)	C10—C11—C12—C15	−60.86 (18)
C2—C3—C4—Cl1	−179.89 (12)	C11—C12—C13—O16'	154.0 (3)
C3—C4—C5—C6	−0.5 (2)	C15—C12—C13—O16'	−87.6 (3)
Cl1—C4—C5—C6	178.75 (12)	C11—C12—C13—O16	67.7 (2)
C4—C5—C6—C1	1.5 (2)	C15—C12—C13—O16	−174.01 (17)
C4—C5—C6—Cl2	−177.99 (12)	C11—C12—C13—C8	−58.8 (2)
C2—C1—C6—C5	−1.3 (2)	C15—C12—C13—C8	59.5 (2)
C7—C1—C6—C5	−177.03 (14)	C7—C8—C13—O16'	−26.6 (4)
C2—C1—C6—Cl2	178.20 (12)	N9—C8—C13—O16'	153.4 (3)
C7—C1—C6—Cl2	2.5 (2)	C7—C8—C13—O16	51.6 (3)
C6—C1—C7—C8	−139.20 (19)	N9—C8—C13—O16	−128.34 (19)
C2—C1—C7—C8	45.3 (3)	C7—C8—C13—C12	−178.55 (18)
C1—C7—C8—N9	5.1 (3)	N9—C8—C13—C12	1.5 (2)
C1—C7—C8—C13	−174.83 (18)	C8—N9—C14—C15	53.4 (2)
C7—C8—N9—C14	121.4 (2)	C10—N9—C14—C15	−63.25 (18)
C13—C8—N9—C14	−58.6 (2)	C13—C12—C15—C14	−63.62 (18)
C7—C8—N9—C10	−122.3 (2)	C11—C12—C15—C14	54.84 (18)
C13—C8—N9—C10	57.6 (2)	N9—C14—C15—C12	6.6 (2)
C8—N9—C10—C11	−59.91 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O16—H16···N9^{i}	0.84	2.05	2.872 (2)	166

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1