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N-Benzyl-2-(2,4-dichlorophenoxy)-acetamide

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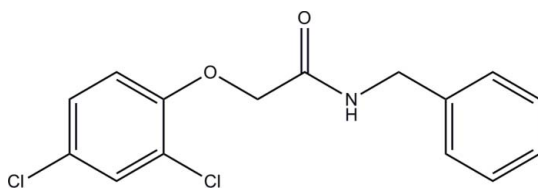
Received 17 July 2008; accepted 13 September 2008

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.039; wR factor = 0.104; data-to-parameter ratio = 17.6.

In the title compound, $\text{C}_{15}\text{H}_{13}\text{Cl}_2\text{NO}_2$, the dihedral angle between the aromatic rings is 27.17 (11)°. In the crystal the molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For related literature, see: Li *et al.* (2008a,b).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{13}\text{Cl}_2\text{NO}_2$
 $M_r = 310.16$
 Monoclinic, $P2_1/c$
 $a = 4.7447$ (6) Å
 $b = 26.821$ (3) Å

$c = 11.3962$ (15) Å
 $\beta = 90.402$ (2)°
 $V = 1450.2$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.45$ mm⁻¹
 $T = 298$ (2) K

$0.30 \times 0.10 \times 0.05$ mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
 $T_{\min} = 0.877$, $T_{\max} = 0.978$

8418 measured reflections
 3254 independent reflections
 2233 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.103$
 $S = 1.03$
 3254 reflections
 185 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.19$ e Å⁻³
 $\Delta\rho_{\min} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N}-\text{H}0\text{A}\cdots\text{O}2^i$	0.83 (2)	2.06 (2)	2.883 (2)	169 (2)

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: WinGX (Farrugia, 1999).

This study was supported by the Science and Technology Key Project of Chongqing Science and Technology Commission, China (grant No. CSTC, 2008 A A1001)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2090).

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supplementary materials

Acta Cryst. (2008). E64, o1968 [doi:10.1107/S1600536808029371]

***N*-Benzyl-2-(2,4-dichlorophenoxy)acetamide**

M.-J. Chen, Y.-W. Fu, W.-L. Dong, Z.-B. Li and H. Zuo

Comment

The structure determination was performed as a part of a project on the interactions of small molecules with proteins. The single-crystal characterization should be valuable to understand such interactions. In our previous papers we reported single crystal structures of *N*-benzyl-2-(2-chloro-4-methylphenoxy)acetamide (Li *et al.*, 2008a) and *N*-benzyl-2-(2,6-dichlorophenoxy)acetamide (Li *et al.*, 2008b). In the title compound, C₁₅H₁₃Cl₂NO₂, all bond lengths and angles are normal. The dihedral angle between the two aryl rings is 27.17 (11)^o. The molecules are connected via N-H...O hydrogen bonding into chains.

Experimental

The solution of 2,4-dichlorophenol (1.0 mmol), *N*-benzyl-2-chloroacetamide (1.1 mmol), K₂CO₃ (1.1 mmol) and CH₃CN (20 ml) was refluxed for 3 h. After completion of the reaction, the solution was cooled; solvent was evaporated under reduced pressure. The residue was poured into water and adjusted the pH to 6–7 with dilute hydrochloric acid (10%) and extracted with ethyl acetate, washed with brine and dried over anhydrous MgSO₄ to obtain the corresponding crude product. The product was purified by column chromatography on silica gel using ethyl acetate as eluent (yield 87%). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid dissolved in ethyl acetate/hexane at room temperatures for 4 days.

Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.97 Å (for CH₂ groups) and 0.96 Å (for CH₃ groups), their isotropic displacement parameters were set to 1.2 times (1.5 times for CH₃ groups) the equivalent displacement parameter of their parent atoms, except the N-H one which was freely refined.

Figures

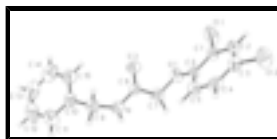


Fig. 1. The molecular structure of the title compound showing displacement ellipsoids drawn at 50% probability level.

***N*-benzyl-2-(2,4-dichlorophenoxy)acetamide**

Crystal data

C₁₅H₁₃Cl₂NO₂

$F_{000} = 640$

supplementary materials

$M_r = 310.16$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 4.7447$ (6) Å

$b = 26.821$ (3) Å

$c = 11.3962$ (15) Å

$\beta = 90.402$ (2)°

$V = 1450.2$ (3) Å³

$Z = 4$

$D_x = 1.421$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2023 reflections

$\theta = 2.4$ – 24.3 °

$\mu = 0.45$ mm⁻¹

$T = 298$ (2) K

Prism, colourless

$0.30 \times 0.10 \times 0.05$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

phi and ω scans

Absorption correction: multi-scan
(PROGRAM? REFERENCE?)

$T_{\min} = 0.878$, $T_{\max} = 0.978$

8418 measured reflections

3254 independent reflections

2233 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\text{max}} = 27.5$ °

$\theta_{\text{min}} = 1.5$ °

$h = -6$ → 6

$k = -26$ → 34

$l = -14$ → 14

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.103$

$S = 1.03$

3254 reflections

185 parameters

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

H atoms treated by a mixture of
independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 0.2337P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.19$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N	-0.5859 (3)	0.13972 (6)	1.13239 (14)	0.0432 (4)
H0A	-0.757 (4)	0.1456 (7)	1.1390 (16)	0.045 (6)*
Cl1	-0.01187 (15)	0.32457 (2)	1.38966 (5)	0.0718 (2)
Cl2	0.22803 (14)	0.39046 (2)	0.95534 (5)	0.0711 (2)
O1	-0.3722 (3)	0.25520 (5)	1.27258 (11)	0.0467 (3)
O2	-0.1562 (3)	0.17031 (5)	1.18000 (13)	0.0533 (4)

C1	-0.0568 (4)	0.32072 (6)	1.23900 (15)	0.0419 (4)
C2	0.0880 (4)	0.35291 (7)	1.16733 (16)	0.0470 (5)
H2A	0.2087	0.3767	1.1991	0.056*
C3	0.0511 (4)	0.34928 (7)	1.04765 (16)	0.0462 (5)
C4	-0.1215 (4)	0.31367 (7)	0.99970 (17)	0.0496 (5)
H4A	-0.1415	0.3112	0.9187	0.059*
C5	-0.2659 (4)	0.28142 (7)	1.07243 (16)	0.0468 (5)
H5A	-0.3834	0.2573	1.0398	0.056*
C6	-0.2379 (4)	0.28461 (6)	1.19306 (15)	0.0386 (4)
C7	-0.5631 (4)	0.21854 (7)	1.23010 (18)	0.0468 (5)
H7A	-0.6842	0.2334	1.1707	0.056*
H7B	-0.6816	0.2075	1.2941	0.056*
C8	-0.4137 (4)	0.17379 (6)	1.17797 (15)	0.0370 (4)
C9	-0.4894 (4)	0.09348 (7)	1.08006 (17)	0.0507 (5)
H9A	-0.2910	0.0966	1.0615	0.061*
H9B	-0.5912	0.0880	1.0071	0.061*
C10	-0.5293 (4)	0.04881 (7)	1.15846 (17)	0.0459 (5)
C11	-0.7149 (5)	0.01174 (9)	1.1278 (2)	0.0726 (7)
H11A	-0.8146	0.0140	1.0574	0.087*
C12	-0.7554 (7)	-0.02898 (10)	1.2005 (3)	0.0908 (9)
H12A	-0.8836	-0.0536	1.1788	0.109*
C13	-0.6107 (7)	-0.03343 (10)	1.3027 (3)	0.0872 (9)
H13A	-0.6395	-0.0608	1.3514	0.105*
C14	-0.4209 (6)	0.00298 (11)	1.3337 (2)	0.0822 (8)
H14A	-0.3190	0.0001	1.4034	0.099*
C15	-0.3801 (5)	0.04402 (9)	1.2619 (2)	0.0640 (6)
H15A	-0.2512	0.0685	1.2838	0.077*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N	0.0327 (9)	0.0426 (9)	0.0543 (10)	0.0032 (7)	0.0025 (7)	-0.0059 (7)
C11	0.1088 (5)	0.0673 (4)	0.0393 (3)	-0.0261 (3)	-0.0006 (3)	-0.0106 (2)
C12	0.0869 (5)	0.0663 (4)	0.0604 (3)	-0.0168 (3)	0.0117 (3)	0.0131 (3)
O1	0.0517 (8)	0.0405 (7)	0.0479 (7)	-0.0087 (6)	0.0045 (6)	-0.0019 (6)
O2	0.0307 (7)	0.0527 (8)	0.0764 (10)	0.0030 (6)	0.0010 (6)	-0.0051 (7)
C1	0.0511 (11)	0.0370 (10)	0.0376 (9)	-0.0001 (8)	0.0002 (8)	-0.0071 (8)
C2	0.0539 (12)	0.0377 (10)	0.0492 (11)	-0.0072 (9)	0.0011 (9)	-0.0065 (8)
C3	0.0506 (11)	0.0407 (10)	0.0475 (11)	0.0004 (9)	0.0053 (9)	0.0029 (9)
C4	0.0584 (13)	0.0515 (12)	0.0388 (10)	0.0030 (10)	-0.0048 (9)	0.0002 (9)
C5	0.0488 (11)	0.0439 (11)	0.0478 (11)	-0.0042 (9)	-0.0083 (9)	-0.0046 (9)
C6	0.0394 (10)	0.0320 (9)	0.0445 (10)	0.0029 (8)	0.0014 (8)	-0.0020 (8)
C7	0.0377 (10)	0.0403 (10)	0.0626 (12)	-0.0041 (8)	0.0075 (9)	-0.0021 (9)
C8	0.0329 (10)	0.0354 (9)	0.0428 (10)	0.0010 (7)	0.0025 (7)	0.0057 (7)
C9	0.0542 (13)	0.0478 (12)	0.0501 (11)	0.0018 (9)	0.0049 (9)	-0.0093 (9)
C10	0.0456 (11)	0.0404 (10)	0.0519 (11)	0.0043 (9)	0.0101 (9)	-0.0087 (9)
C11	0.0747 (17)	0.0613 (15)	0.0816 (17)	-0.0152 (13)	-0.0013 (13)	-0.0055 (13)
C12	0.098 (2)	0.0560 (16)	0.119 (3)	-0.0247 (15)	0.020 (2)	-0.0025 (16)

supplementary materials

C13	0.103 (2)	0.0540 (16)	0.105 (2)	0.0148 (16)	0.0368 (19)	0.0151 (15)
C14	0.096 (2)	0.0809 (19)	0.0693 (17)	0.0239 (17)	0.0031 (14)	0.0134 (15)
C15	0.0697 (15)	0.0590 (14)	0.0632 (14)	0.0012 (11)	-0.0021 (12)	-0.0024 (11)

Geometric parameters (Å, °)

N—C8	1.329 (2)	C7—C8	1.517 (2)
N—C9	1.451 (2)	C7—H7A	0.9700
N—H0A	0.83 (2)	C7—H7B	0.9700
C11—C1	1.7318 (18)	C9—C10	1.507 (3)
C12—C3	1.7448 (19)	C9—H9A	0.9700
O1—C6	1.363 (2)	C9—H9B	0.9700
O1—C7	1.420 (2)	C10—C11	1.372 (3)
O2—C8	1.225 (2)	C10—C15	1.377 (3)
C1—C2	1.376 (3)	C11—C12	1.385 (4)
C1—C6	1.394 (2)	C11—H11A	0.9300
C2—C3	1.377 (3)	C12—C13	1.353 (4)
C2—H2A	0.9300	C12—H12A	0.9300
C3—C4	1.369 (3)	C13—C14	1.373 (4)
C4—C5	1.383 (3)	C13—H13A	0.9300
C4—H4A	0.9300	C14—C15	1.386 (3)
C5—C6	1.383 (2)	C14—H14A	0.9300
C5—H5A	0.9300	C15—H15A	0.9300
C8—N—C9	123.59 (16)	O2—C8—N	124.41 (16)
C8—N—H0A	115.6 (14)	O2—C8—C7	121.43 (16)
C9—N—H0A	120.7 (14)	N—C8—C7	114.16 (15)
C6—O1—C7	118.32 (14)	N—C9—C10	113.22 (16)
C2—C1—C6	121.47 (17)	N—C9—H9A	108.9
C2—C1—C11	119.52 (14)	C10—C9—H9A	108.9
C6—C1—C11	119.00 (14)	N—C9—H9B	108.9
C1—C2—C3	118.88 (17)	C10—C9—H9B	108.9
C1—C2—H2A	120.6	H9A—C9—H9B	107.7
C3—C2—H2A	120.6	C11—C10—C15	118.4 (2)
C4—C3—C2	121.07 (18)	C11—C10—C9	120.5 (2)
C4—C3—C12	119.33 (15)	C15—C10—C9	121.05 (19)
C2—C3—C12	119.60 (15)	C10—C11—C12	120.7 (3)
C3—C4—C5	119.63 (18)	C10—C11—H11A	119.7
C3—C4—H4A	120.2	C12—C11—H11A	119.7
C5—C4—H4A	120.2	C13—C12—C11	120.9 (3)
C6—C5—C4	120.84 (18)	C13—C12—H12A	119.6
C6—C5—H5A	119.6	C11—C12—H12A	119.6
C4—C5—H5A	119.6	C12—C13—C14	119.1 (3)
O1—C6—C5	125.67 (16)	C12—C13—H13A	120.5
O1—C6—C1	116.25 (15)	C14—C13—H13A	120.5
C5—C6—C1	118.09 (17)	C13—C14—C15	120.5 (3)
O1—C7—C8	112.50 (14)	C13—C14—H14A	119.8
O1—C7—H7A	109.1	C15—C14—H14A	119.8
C8—C7—H7A	109.1	C10—C15—C14	120.4 (2)
O1—C7—H7B	109.1	C10—C15—H15A	119.8

C8—C7—H7B	109.1	C14—C15—H15A	119.8
H7A—C7—H7B	107.8		
C6—C1—C2—C3	0.3 (3)	C9—N—C8—O2	0.7 (3)
C11—C1—C2—C3	179.74 (15)	C9—N—C8—C7	-178.70 (16)
C1—C2—C3—C4	-1.4 (3)	O1—C7—C8—O2	3.5 (3)
C1—C2—C3—C12	178.90 (14)	O1—C7—C8—N	-177.05 (15)
C2—C3—C4—C5	1.3 (3)	C8—N—C9—C10	103.3 (2)
C12—C3—C4—C5	-178.97 (15)	N—C9—C10—C11	113.8 (2)
C3—C4—C5—C6	-0.1 (3)	N—C9—C10—C15	-66.5 (3)
C7—O1—C6—C5	-1.4 (2)	C15—C10—C11—C12	1.4 (3)
C7—O1—C6—C1	178.78 (15)	C9—C10—C11—C12	-179.0 (2)
C4—C5—C6—O1	179.23 (17)	C10—C11—C12—C13	-0.8 (4)
C4—C5—C6—C1	-1.0 (3)	C11—C12—C13—C14	-0.3 (4)
C2—C1—C6—O1	-179.29 (16)	C12—C13—C14—C15	0.7 (4)
C11—C1—C6—O1	1.3 (2)	C11—C10—C15—C14	-0.9 (3)
C2—C1—C6—C5	0.9 (3)	C9—C10—C15—C14	179.4 (2)
C11—C1—C6—C5	-178.57 (14)	C13—C14—C15—C10	-0.1 (4)
C6—O1—C7—C8	75.3 (2)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N-H0A\cdots O2^i$	0.83 (2)	2.06 (2)	2.883 (2)	169 (2)

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

Fig. 1

