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N-(2,4-Dichlorophenyl)-2-nitrobenzamide

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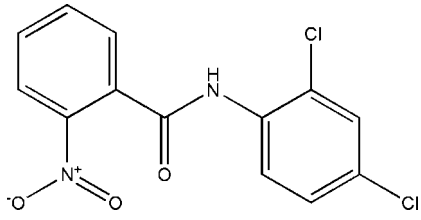
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.086; data-to-parameter ratio = 20.2.

The geometric parameters of the title compound, $C_{13}H_8Cl_2N_2O_3$, are in the usual ranges. The dihedral angle between the two aromatic rings is 78.33 (3)°. The crystal structure is stabilized by an N—H···O hydrogen bond.

Related literature

For related literature, see: Igawa *et al.* (1999); Jackson *et al.* (1994); Makino *et al.* (2001, 2003); Manley *et al.* (2002); Zhichkin *et al.* (2007); Capdeville *et al.* (2002); Ho *et al.* (2002).



Experimental

Crystal data

$C_{13}H_8Cl_2N_2O_3$
M_r = 311.11
Monoclinic, $P2_1/n$
a = 11.4761 (8) Å
b = 8.8577 (3) Å
c = 13.8105 (8) Å
β = 106.893 (5)°
V = 1343.3 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 173 (2) K
0.33 × 0.30 × 0.25 mm

Data collection

Stoe IPDSII two-circle-diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.855, T_{max} = 0.887
23274 measured reflections
3758 independent reflections
3425 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.086
S = 1.03
3758 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.863 (19)	2.172 (18)	2.9401 (14)	148.1 (16)

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: IM2046).

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supplementary materials

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N-(2,4-Dichlorophenyl)-2-nitrobenzamide

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Comment

The benzanilide core is present in compounds with such a wide range of biological activities that it has been called a privileged structural motif. Benzanilides serve as intermediates towards benzothiadiazin-4-ones (Makino *et al.*, 2003), quinazoline-2,4-diones (Makino *et al.*, 2001) and benzodiazepine-2,5-diones (Ho *et al.*, 2002). 2,3-disubstituted 3*H*-quinazoline-4-ones act as 110δ kinase inhibitors (Zhichkin *et al.*, 2007). Benzanilides have established their efficacy as central elements of ligands that bind to a wide variety of receptor types. Thus benzanilides containing aminoalkyl groups originally designed as peptidomimetics, have been incorporated in an Arg-Gly-Asp cyclic peptide yielding a high affinity GPIIb/IIIa ligand (Jackson *et al.*, 1994). Imatinib, a 2-phenylaminopyrimidine derivative with an additional benzanilide substituent, is a drug used to treat certain kinds of cancer by inhibiting a number of tyrosine kinase enzymes (Capdeville *et al.*, 2002). Pyridylmethyl containing benzanilides are vascular endothelial growth factor receptor and tyrosine kinase inhibitors (Manley *et al.*, 2002). Furthermore, benzamides have been reported to exhibit activities as acetyl-CoA carboxylase and farnesyl transferase inhibitors (Igawa *et al.*, 1999)

Geometric parameters of the title compound are in the usual ranges. The dihedral angle between the two aromatic rings is 78.33 (3)°. The nitro group is slightly bent out of the plane of the phenyl ring to which it is attached by 4.2 (3)°. The crystal structure is stabilized by an N—H···O hydrogen bond.

Experimental

A mixture of 2,4-dichloroaniline (10.0 g, 61.74 mmol), 2-nitrobenzoyl chloride (10 ml, 86.9 mmol), and pyridine (20 ml) was left at 25 °C for 15 h. Water (100 ml) was then added, and the resulting precipitates were collected. Recrystallization of the precipitates from benzene gave 15.74 g (82%) of title compound as yellow needles.

Refinement

All H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C)] using a riding model with C—H = 0.95 Å. The amino H atom was freely refined.

Figures

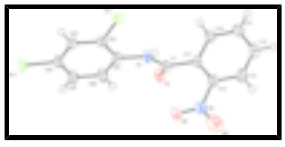


Fig. 1. Molecular structure of title compound with displacement ellipsoids at the 50% probability level.

N-(2,4-Dichlorophenyl)-2-nitrobenzamide

Crystal data

$C_{13}H_8Cl_2N_2O_3$	F_{000} = 632
M_r = 311.11	D_x = 1.538 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 23725 reflections
a = 11.4761 (8) Å	θ = 3.6–29.7º
b = 8.8577 (3) Å	μ = 0.49 mm^{-1}
c = 13.8105 (8) Å	T = 173 (2) K
β = 106.893 (5)º	Block, light brown
V = 1343.3 (1) Å^3	0.33 × 0.30 × 0.25 mm
Z = 4	

Data collection

STOE IPDS II two-circle-diffractometer	3758 independent reflections
Radiation source: fine-focus sealed tube	3425 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 173(2) K	θ_{max} = 29.6º
ω scans	θ_{min} = 3.6º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	h = −15→15
T_{min} = 0.855, T_{max} = 0.887	k = −12→11
23274 measured reflections	l = −19→19

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.5969P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.086	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.03	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
3758 reflections	$\Delta\rho_{min}$ = −0.45 e Å^{-3}
186 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0125 (15)
Secondary atom site location: difference Fourier map	

Special details

Experimental. ;

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}
Cl1	0.49367 (3)	0.69203 (4)	0.65360 (2)	0.03091 (9)
Cl2	0.25833 (4)	0.60345 (5)	0.26026 (2)	0.04686 (12)
N1	0.30883 (10)	0.48700 (12)	0.69438 (7)	0.0248 (2)
H1	0.3364 (17)	0.565 (2)	0.7309 (14)	0.037 (4)*
N2	0.10801 (12)	0.56153 (15)	0.84036 (9)	0.0367 (3)
O1	0.20242 (9)	0.26735 (10)	0.69472 (6)	0.0296 (2)
O2	0.07693 (9)	0.54611 (13)	0.74857 (7)	0.0374 (2)
O3	0.05376 (16)	0.6415 (2)	0.88434 (11)	0.0858 (6)
C1	0.25772 (11)	0.37847 (13)	0.73830 (8)	0.0225 (2)
C11	0.28609 (11)	0.39697 (13)	0.85223 (8)	0.0221 (2)
C12	0.21713 (12)	0.48132 (14)	0.90077 (9)	0.0264 (2)
C13	0.24700 (14)	0.49206 (17)	1.00569 (10)	0.0339 (3)
H13	0.1985	0.5508	1.0367	0.041*
C14	0.34849 (14)	0.41581 (17)	1.06428 (9)	0.0342 (3)
H14	0.3701	0.4224	1.1360	0.041*
C15	0.41841 (13)	0.32998 (17)	1.01840 (10)	0.0337 (3)
H15	0.4875	0.2771	1.0588	0.040*
C16	0.38771 (12)	0.32081 (15)	0.91294 (9)	0.0294 (3)
H16	0.4365	0.2621	0.8822	0.035*
C21	0.29876 (11)	0.50223 (13)	0.59010 (8)	0.0233 (2)
C22	0.37878 (10)	0.60066 (14)	0.56190 (8)	0.0233 (2)
C23	0.36844 (12)	0.63043 (15)	0.46057 (9)	0.0289 (3)
H23	0.4227	0.6984	0.4425	0.035*
C24	0.27715 (12)	0.55842 (16)	0.38694 (9)	0.0299 (3)
C25	0.19979 (13)	0.45599 (17)	0.41143 (9)	0.0346 (3)
H25	0.1399	0.4049	0.3597	0.041*
C26	0.21057 (13)	0.42819 (17)	0.51313 (9)	0.0334 (3)
H26	0.1573	0.3580	0.5304	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02629 (15)	0.03753 (17)	0.02775 (15)	−0.00647 (11)	0.00601 (11)	−0.00133 (11)
Cl2	0.0584 (2)	0.0652 (3)	0.01816 (15)	0.01553 (19)	0.01304 (14)	0.00884 (14)
N1	0.0323 (5)	0.0260 (5)	0.0161 (4)	−0.0068 (4)	0.0070 (4)	−0.0029 (4)
N2	0.0388 (6)	0.0402 (6)	0.0309 (6)	0.0145 (5)	0.0097 (5)	0.0030 (5)
O1	0.0416 (5)	0.0241 (4)	0.0213 (4)	−0.0075 (4)	0.0065 (3)	−0.0017 (3)
O2	0.0344 (5)	0.0462 (6)	0.0283 (5)	0.0070 (4)	0.0039 (4)	0.0092 (4)
O3	0.0848 (11)	0.1187 (14)	0.0503 (8)	0.0724 (11)	0.0140 (7)	−0.0108 (8)
C1	0.0268 (5)	0.0227 (5)	0.0177 (5)	0.0005 (4)	0.0058 (4)	0.0002 (4)
C11	0.0270 (5)	0.0215 (5)	0.0176 (5)	−0.0025 (4)	0.0064 (4)	−0.0004 (4)
C12	0.0315 (6)	0.0267 (5)	0.0209 (5)	0.0042 (4)	0.0077 (4)	0.0022 (4)
C13	0.0436 (7)	0.0380 (7)	0.0225 (6)	0.0057 (6)	0.0131 (5)	−0.0021 (5)
C14	0.0439 (7)	0.0394 (7)	0.0175 (5)	0.0000 (6)	0.0063 (5)	−0.0003 (5)
C15	0.0346 (6)	0.0385 (7)	0.0229 (6)	0.0047 (5)	0.0003 (5)	0.0009 (5)
C16	0.0301 (6)	0.0333 (6)	0.0232 (5)	0.0047 (5)	0.0052 (4)	−0.0029 (5)
C21	0.0281 (5)	0.0250 (5)	0.0171 (5)	−0.0002 (4)	0.0069 (4)	−0.0006 (4)
C22	0.0233 (5)	0.0269 (5)	0.0201 (5)	0.0024 (4)	0.0066 (4)	0.0000 (4)
C23	0.0313 (6)	0.0347 (6)	0.0242 (5)	0.0039 (5)	0.0137 (5)	0.0045 (5)
C24	0.0353 (6)	0.0386 (7)	0.0166 (5)	0.0106 (5)	0.0089 (4)	0.0029 (4)
C25	0.0386 (7)	0.0424 (7)	0.0191 (5)	−0.0021 (6)	0.0027 (5)	−0.0033 (5)
C26	0.0378 (7)	0.0394 (7)	0.0208 (5)	−0.0111 (6)	0.0052 (5)	−0.0017 (5)

Geometric parameters (Å, °)

Cl1—C22	1.7398 (12)	C14—C15	1.385 (2)
Cl2—C24	1.7455 (12)	C14—H14	0.9500
N1—C1	1.3576 (15)	C15—C16	1.3977 (17)
N1—C21	1.4174 (14)	C15—H15	0.9500
N1—H1	0.863 (19)	C16—H16	0.9500
N2—O3	1.2155 (17)	C21—C26	1.3996 (17)
N2—O2	1.2207 (15)	C21—C22	1.4011 (16)
N2—C12	1.4703 (17)	C22—C23	1.3947 (16)
O1—C1	1.2295 (14)	C23—C24	1.3854 (19)
C1—C11	1.5201 (15)	C23—H23	0.9500
C11—C12	1.3937 (16)	C24—C25	1.378 (2)
C11—C16	1.3963 (17)	C25—C26	1.3956 (17)
C12—C13	1.3919 (16)	C25—H25	0.9500
C13—C14	1.385 (2)	C26—H26	0.9500
C13—H13	0.9500		
C1—N1—C21	127.09 (10)	C16—C15—H15	119.9
C1—N1—H1	116.2 (12)	C11—C16—C15	120.75 (12)
C21—N1—H1	115.2 (12)	C11—C16—H16	119.6
O3—N2—O2	123.13 (13)	C15—C16—H16	119.6
O3—N2—C12	118.25 (12)	C26—C21—C22	117.91 (11)
O2—N2—C12	118.61 (11)	C26—C21—N1	123.68 (11)

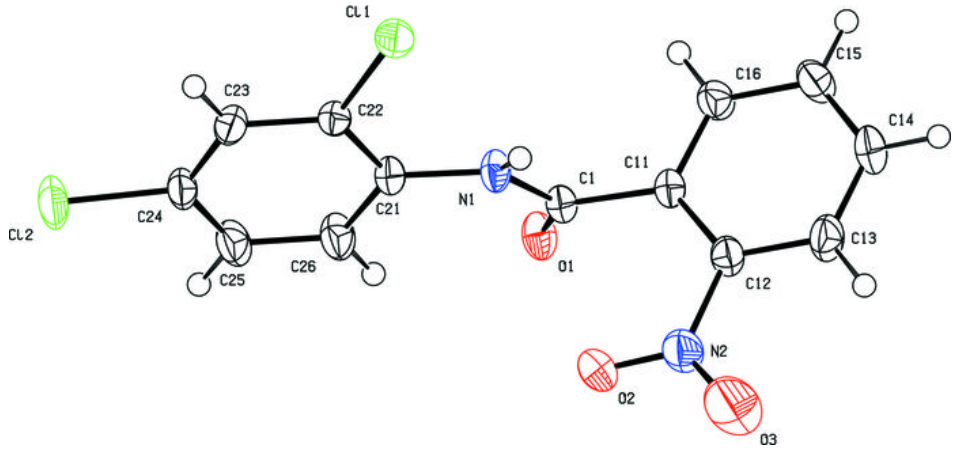
O1—C1—N1	125.22 (10)	C22—C21—N1	118.37 (10)
O1—C1—C11	121.18 (10)	C23—C22—C21	121.67 (11)
N1—C1—C11	113.31 (10)	C23—C22—Cl1	117.90 (10)
C12—C11—C16	117.52 (10)	C21—C22—Cl1	120.43 (9)
C12—C11—C1	125.09 (10)	C24—C23—C22	118.37 (12)
C16—C11—C1	117.37 (10)	C24—C23—H23	120.8
C13—C12—C11	122.34 (11)	C22—C23—H23	120.8
C13—C12—N2	117.98 (11)	C25—C24—C23	121.77 (11)
C11—C12—N2	119.68 (10)	C25—C24—Cl2	119.70 (10)
C14—C13—C12	119.05 (12)	C23—C24—Cl2	118.52 (10)
C14—C13—H13	120.5	C24—C25—C26	119.21 (12)
C12—C13—H13	120.5	C24—C25—H25	120.4
C15—C14—C13	120.06 (12)	C26—C25—H25	120.4
C15—C14—H14	120.0	C25—C26—C21	120.98 (12)
C13—C14—H14	120.0	C25—C26—H26	119.5
C14—C15—C16	120.29 (12)	C21—C26—H26	119.5
C14—C15—H15	119.9		
C21—N1—C1—O1	6.7 (2)	C12—C11—C16—C15	−0.16 (19)
C21—N1—C1—C11	−179.36 (11)	C1—C11—C16—C15	−178.82 (12)
O1—C1—C11—C12	−96.77 (15)	C14—C15—C16—C11	−0.3 (2)
N1—C1—C11—C12	89.02 (15)	C1—N1—C21—C26	16.0 (2)
O1—C1—C11—C16	81.78 (15)	C1—N1—C21—C22	−166.17 (12)
N1—C1—C11—C16	−92.43 (13)	C26—C21—C22—C23	2.93 (19)
C16—C11—C12—C13	0.49 (19)	N1—C21—C22—C23	−175.00 (11)
C1—C11—C12—C13	179.04 (12)	C26—C21—C22—Cl1	−178.00 (10)
C16—C11—C12—N2	−178.94 (12)	N1—C21—C22—Cl1	4.08 (16)
C1—C11—C12—N2	−0.40 (19)	C21—C22—C23—C24	−0.81 (18)
O3—N2—C12—C13	4.9 (2)	Cl1—C22—C23—C24	−179.91 (10)
O2—N2—C12—C13	−175.91 (14)	C22—C23—C24—C25	−2.0 (2)
O3—N2—C12—C11	−175.68 (17)	C22—C23—C24—Cl2	176.39 (9)
O2—N2—C12—C11	3.6 (2)	C23—C24—C25—C26	2.5 (2)
C11—C12—C13—C14	−0.3 (2)	Cl2—C24—C25—C26	−175.85 (11)
N2—C12—C13—C14	179.13 (13)	C24—C25—C26—C21	−0.2 (2)
C12—C13—C14—C15	−0.2 (2)	C22—C21—C26—C25	−2.4 (2)
C13—C14—C15—C16	0.5 (2)	N1—C21—C26—C25	175.42 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.863 (19)	2.172 (18)	2.9401 (14)	148.1 (16)

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+3/2.

Fig. 1


CL1
C23
C22
C15
C16
C14
C11
C1
N1
C21
C24
CL2
C25
C26
O1
C13
C12
N2
O2
O3