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1-Cyano-*N*-(2,4,5-trichlorophenyl)cyclopropane-1-carboxamide

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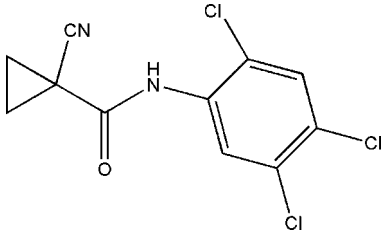
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.107; data-to-parameter ratio = 13.8.

In the title compound, $C_{11}H_7Cl_3N_3O$, the dihedral angle between the benzene and cyclopropane rings is 85.8 (2)°. In the crystal, molecules are linked by C—H···O interactions, generating $C(5)$ chains propagating in the a-axis direction.

Related literature

For the synthesis, see: Liu *et al.* (2007). For the biological activity of related compounds, see: Liu *et al.* (2009).



Experimental

Crystal data

$C_{11}H_7Cl_3N_2O$
M_r = 289.54
Triclinic, $P\overline{1}$
a = 6.0068 (18) Å
b = 7.420 (2) Å
c = 14.047 (4) Å
α = 77.531 (5)°
β = 86.958 (5)°
γ = 84.483 (5)°
V = 608.1 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 294 K
0.24 × 0.22 × 0.18 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.614, T_{max} = 1.000
3103 measured reflections
2130 independent reflections
1619 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.107
S = 1.04
2130 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10B···O1^{i}	0.97	2.56	3.439 (3)	151

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5931).

References

Liu, X. H., Chen, P. Q., Wang, B. L., Li, Y. H., Wang, S. H. & Li, Z. M. (2007). *Bioorg. Med. Chem. Lett.* **17**, 3784–3788.
Liu, X. H., Shi, Y. X., Ma, Y., Zhang, C. Y., Dong, W. L., Li, P., Wang, B. L., li, B. J. & li, Z. M. (2009). *Eur. J. Med. Chem.* **44**, 2782–2786.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o1940 [doi:10.1107/S1600536811026225]

1-Cyano-*N*-(2,4,5-trichlorophenyl)cyclopropane-1-carboxamide

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S1. Comment

Many cyclopropane compound exhibit good biological activity such as KARI (Liu *et al.*, 2007; Liu *et al.*, 2009). In continuation of this work, the title compound, (I), a 1-cyano-carboxamide derivatives had been synthesized. The strucuture was confirmed by X-ray crstallography.

Single-crystal X-ray diffraction analysis reveals that the title compound crystallizes in the triclinic space group $P\bar{1}$ (Fig. 1). As shown in Fig. 2, the crystal structure is stabilized by weak C-H···O intermolecular interactions.

S2. Experimental

The title compound was prepared according to the literature procedures (Liu *et al.*, 2007). Colourless prisms of (I) were grown from slow evaporation of ethanol solution at room temperature.

S3. Refinement

All the H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

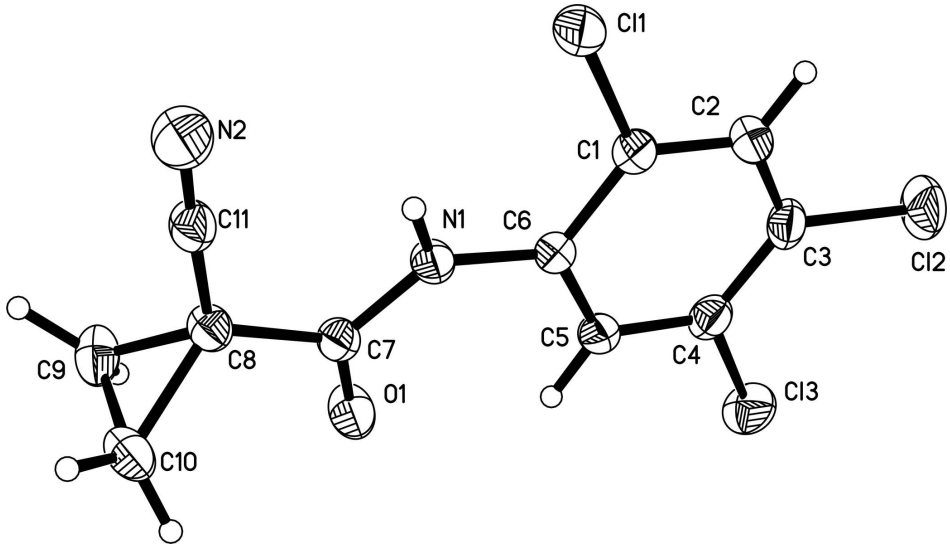

Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

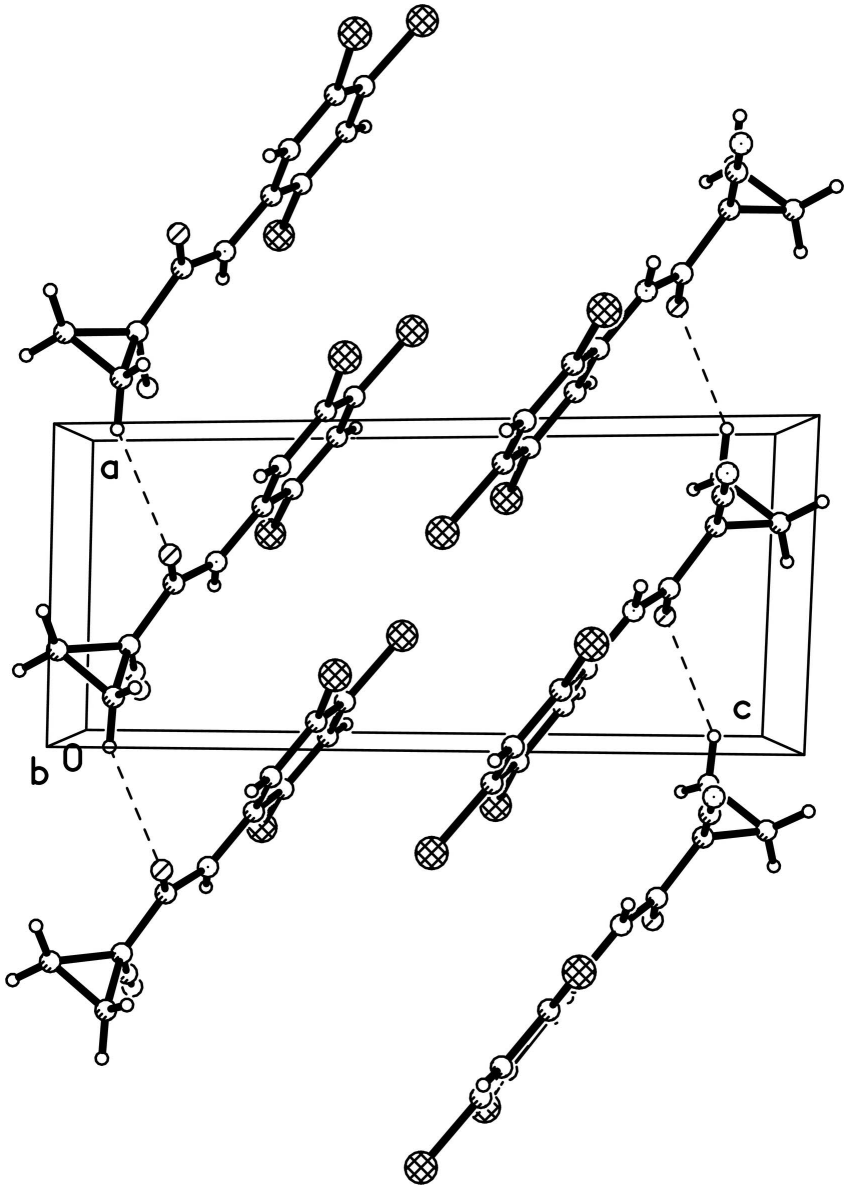

Figure 2

The crystal packing for (I).

1-Cyano-*N*-(2,4,5-trichlorophenyl)cyclopropane-1-carboxamide

Crystal data

$C_{11}H_7Cl_3N_2O$
$M_r = 289.54$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.0068$ (18) Å
$b = 7.420$ (2) Å
$c = 14.047$ (4) Å
$\alpha = 77.531$ (5)°
$\beta = 86.958$ (5)°
$\gamma = 84.483$ (5)°
$V = 608.1$ (3) Å^3
$Z = 2$
$F(000) = 292$
$D_x = 1.581$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1405 reflections
$\theta = 3.0$–26.2°
$\mu = 0.74$ mm^{-1}

T = 294 K
Prism, colorless

0.24 × 0.22 × 0.18 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.614, T_{max} = 1.000

3103 measured reflections
2130 independent reflections
1619 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°, θ_{min} = 1.5°
h = −6→7
k = −8→7
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.107
S = 1.04
2130 reflections
154 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
$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 0.1114P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.32398 (14)	0.92602 (9)	0.72571 (5)	0.0647 (3)
Cl2	−0.33513 (13)	0.75928 (12)	0.52559 (6)	0.0763 (3)
Cl3	−0.21699 (12)	0.33282 (11)	0.61532 (6)	0.0662 (3)
O1	0.4025 (3)	0.2145 (2)	0.84621 (14)	0.0576 (5)
N1	0.4219 (3)	0.5242 (2)	0.79194 (14)	0.0414 (5)
H1	0.4980	0.6139	0.7971	0.050*
N2	0.8457 (4)	0.6623 (3)	0.90380 (19)	0.0669 (7)
C1	0.1788 (4)	0.7600 (3)	0.69152 (17)	0.0445 (6)
C2	0.0042 (4)	0.8156 (4)	0.62960 (17)	0.0511 (6)
H2	−0.0315	0.9410	0.6044	0.061*
C3	−0.1181 (4)	0.6857 (4)	0.60479 (17)	0.0487 (6)
C4	−0.0613 (4)	0.4991 (4)	0.64223 (17)	0.0456 (6)
C5	0.1165 (4)	0.4420 (3)	0.70298 (17)	0.0416 (6)
H5	0.1535	0.3162	0.7265	0.050*

C6	0.2406 (4)	0.5713 (3)	0.72921 (16)	0.0384 (5)
C7	0.4916 (4)	0.3549 (3)	0.84540 (16)	0.0389 (5)
C8	0.6910 (4)	0.3493 (3)	0.90622 (17)	0.0399 (5)
C9	0.7029 (4)	0.2025 (4)	1.00043 (19)	0.0541 (7)
H9A	0.7702	0.2326	1.0557	0.065*
H9B	0.5788	0.1257	1.0172	0.065*
C10	0.8503 (4)	0.1735 (3)	0.9183 (2)	0.0542 (7)
H10A	0.8171	0.0790	0.8844	0.065*
H10B	1.0084	0.1859	0.9229	0.065*
C11	0.7815 (4)	0.5227 (3)	0.90572 (18)	0.0448 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0982 (6)	0.0340 (4)	0.0636 (4)	−0.0070 (3)	−0.0273 (4)	−0.0075 (3)
Cl2	0.0624 (5)	0.0970 (6)	0.0646 (5)	0.0174 (4)	−0.0291 (4)	−0.0110 (4)
Cl3	0.0541 (4)	0.0776 (5)	0.0773 (5)	−0.0072 (3)	−0.0193 (3)	−0.0347 (4)
O1	0.0623 (12)	0.0366 (10)	0.0747 (12)	−0.0121 (8)	−0.0290 (9)	−0.0040 (9)
N1	0.0473 (11)	0.0293 (10)	0.0494 (11)	−0.0057 (8)	−0.0149 (9)	−0.0083 (9)
N2	0.0657 (15)	0.0534 (15)	0.0857 (18)	−0.0150 (12)	−0.0214 (13)	−0.0152 (13)
C1	0.0563 (15)	0.0387 (13)	0.0391 (13)	−0.0025 (11)	−0.0064 (11)	−0.0093 (10)
C2	0.0622 (17)	0.0453 (15)	0.0418 (14)	0.0097 (12)	−0.0073 (12)	−0.0054 (12)
C3	0.0449 (14)	0.0644 (17)	0.0354 (13)	0.0079 (12)	−0.0098 (10)	−0.0111 (12)
C4	0.0426 (14)	0.0563 (15)	0.0419 (13)	−0.0019 (11)	−0.0058 (11)	−0.0193 (12)
C5	0.0447 (14)	0.0379 (13)	0.0445 (13)	0.0014 (10)	−0.0099 (11)	−0.0137 (11)
C6	0.0420 (13)	0.0376 (13)	0.0364 (12)	0.0018 (10)	−0.0060 (10)	−0.0107 (10)
C7	0.0384 (13)	0.0365 (13)	0.0429 (13)	−0.0024 (10)	−0.0065 (10)	−0.0095 (10)
C8	0.0366 (13)	0.0361 (12)	0.0470 (14)	−0.0044 (10)	−0.0061 (10)	−0.0070 (10)
C9	0.0567 (16)	0.0532 (16)	0.0497 (15)	−0.0139 (12)	−0.0155 (13)	0.0026 (12)
C10	0.0459 (15)	0.0420 (14)	0.0719 (18)	0.0037 (11)	−0.0141 (13)	−0.0063 (13)
C11	0.0405 (13)	0.0430 (14)	0.0517 (14)	−0.0039 (11)	−0.0124 (11)	−0.0090 (11)

Geometric parameters (Å, º)

Cl1—C1	1.736 (2)	C4—C5	1.379 (3)
Cl2—C3	1.729 (2)	C5—C6	1.390 (3)
Cl3—C4	1.732 (2)	C5—H5	0.9300
O1—C7	1.213 (3)	C7—C8	1.500 (3)
N1—C7	1.357 (3)	C8—C11	1.442 (3)
N1—C6	1.407 (3)	C8—C9	1.522 (3)
N1—H1	0.8600	C8—C10	1.525 (3)
N2—C11	1.134 (3)	C9—C10	1.456 (4)
C1—C2	1.373 (3)	C9—H9A	0.9700
C1—C6	1.407 (3)	C9—H9B	0.9700
C2—C3	1.378 (4)	C10—H10A	0.9700
C2—H2	0.9300	C10—H10B	0.9700
C3—C4	1.386 (4)		

C7—N1—C6	128.11 (18)	O1—C7—C8	120.4 (2)
C7—N1—H1	115.9	N1—C7—C8	115.52 (18)
C6—N1—H1	115.9	C11—C8—C7	117.5 (2)
C2—C1—C6	121.4 (2)	C11—C8—C9	117.5 (2)
C2—C1—Cl1	119.39 (19)	C7—C8—C9	116.26 (19)
C6—C1—Cl1	119.17 (18)	C11—C8—C10	118.7 (2)
C1—C2—C3	120.1 (2)	C7—C8—C10	116.0 (2)
C1—C2—H2	120.0	C9—C8—C10	57.10 (17)
C3—C2—H2	120.0	C10—C9—C8	61.57 (16)
C2—C3—C4	119.2 (2)	C10—C9—H9A	117.6
C2—C3—Cl2	119.1 (2)	C8—C9—H9A	117.6
C4—C3—Cl2	121.6 (2)	C10—C9—H9B	117.6
C5—C4—C3	121.1 (2)	C8—C9—H9B	117.6
C5—C4—Cl3	118.6 (2)	H9A—C9—H9B	114.7
C3—C4—Cl3	120.33 (19)	C9—C10—C8	61.33 (17)
C4—C5—C6	120.4 (2)	C9—C10—H10A	117.6
C4—C5—H5	119.8	C8—C10—H10A	117.6
C6—C5—H5	119.8	C9—C10—H10B	117.6
C5—C6—C1	117.8 (2)	C8—C10—H10B	117.6
C5—C6—N1	123.8 (2)	H10A—C10—H10B	114.7
C1—C6—N1	118.4 (2)	N2—C11—C8	177.5 (3)
O1—C7—N1	124.1 (2)		

C6—C1—C2—C3	1.5 (4)	C7—N1—C6—C1	171.1 (2)
Cl1—C1—C2—C3	−177.48 (19)	C6—N1—C7—O1	0.1 (4)
C1—C2—C3—C4	−0.7 (4)	C6—N1—C7—C8	−179.6 (2)
C1—C2—C3—Cl2	−179.28 (19)	O1—C7—C8—C11	−176.9 (2)
C2—C3—C4—C5	−0.6 (4)	N1—C7—C8—C11	2.9 (3)
Cl2—C3—C4—C5	178.01 (18)	O1—C7—C8—C9	−30.1 (3)
C2—C3—C4—Cl3	178.07 (18)	N1—C7—C8—C9	149.7 (2)
Cl2—C3—C4—Cl3	−3.4 (3)	O1—C7—C8—C10	34.3 (3)
C3—C4—C5—C6	1.0 (4)	N1—C7—C8—C10	−146.0 (2)
Cl3—C4—C5—C6	−177.66 (18)	C11—C8—C9—C10	−107.9 (2)
C4—C5—C6—C1	−0.2 (3)	C7—C8—C9—C10	105.3 (2)
C4—C5—C6—N1	179.0 (2)	C11—C8—C10—C9	105.8 (2)
C2—C1—C6—C5	−1.0 (3)	C7—C8—C10—C9	−105.7 (2)
Cl1—C1—C6—C5	177.93 (17)	C7—C8—C11—N2	14 (7)
C2—C1—C6—N1	179.7 (2)	C9—C8—C11—N2	−132 (7)
Cl1—C1—C6—N1	−1.3 (3)	C10—C8—C11—N2	162 (6)
C7—N1—C6—C5	−8.1 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*B*···O1^{i}	0.97	2.56	3.439 (3)	151

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