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n-Butyl 2-(3-chloro-1,2-dihydropyrazin-2-ylidene)-2-cyanoacetate

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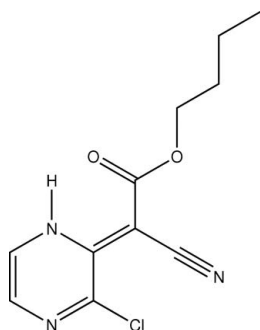
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 Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; disorder in main residue; R factor = 0.047; wR factor = 0.156; data-to-parameter ratio = 10.9.

The title compound, $\text{C}_{11}\text{H}_{12}\text{ClN}_3\text{O}_2$, is essentially planar except for the *n*-butoxy group [r.m.s. deviation from the least-squares plane = 0.0131 (1) Å for 11 non-H atoms]. An intramolecular $\text{N}-\text{H}\cdots\text{O}$ interaction results in the formation of an $S(6)$ ring. The *n*-butoxy chain in the molecule is disordered over two sets of sites of equal occupancy.

Related literature

For applications of this class of compounds, see: Matter *et al.* (2005); Kaliszán *et al.* (1985); Petruszewicz *et al.* (1992, 1993, 1995). For pyrazinyl-pyrazylidene tautomerism, see: Pilarski *et al.* (1984). For related structures, see: Vishweshwar *et al.* (2000); Wardell *et al.* (2006). For the synthesis, see: Pilarski & Foks (1981, 1982).



Experimental

Crystal data

 $\text{C}_{11}\text{H}_{12}\text{ClN}_3\text{O}_2$
 $M_r = 253.69$
 Monoclinic, C_c
 $a = 4.918$ (3) Å
 $b = 25.642$ (7) Å

 $c = 10.573$ (4) Å
 $\beta = 95.80$ (3)°
 $V = 1326.7$ (9) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

 $\mu = 0.28$ mm⁻¹
 $T = 120$ K

 $0.57 \times 0.11 \times 0.07$ mm

Data collection

 Oxford Diffraction KM-4/Xcalibur diffractometer with a Sapphire2 (large Be window) detector
 Absorption correction: Gaussian (*CrysAlis Pro*; Oxford

 Diffraction, 2007)
 $T_{\min} = 0.923$, $T_{\max} = 0.987$
 4629 measured reflections
 1687 independent reflections
 1219 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.156$
 $S = 1.04$
 1687 reflections
 154 parameters
 1 restraint

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.24$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³
 Absolute structure: Flack (1983), 466 Friedel pairs
 Flack parameter: 0.05 (18)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2B}\cdots\text{O1}$	0.87 (2)	1.96 (5)	2.632 (6)	133 (6)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2612).

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supplementary materials

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***n*-Butyl 2-(3-chloro-1,2-dihydropyrazin-2-ylidene)-2-cyanoacetate**

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Comment

Heterocyclic compounds with active methylene moiety are known to have antiinflammatory (Petrušewicz *et al.*, 1995), analgesic (Kaliszan *et al.*, 1985) and large number of other pharmacological activities (Petrušewicz *et al.*, 1992). Numerous scientific publications confirm that pyrazine derivatives, obtained by nucleophilic substitution of chlorine atom in the pyrazine ring system with active methylene compound, possess above mentioned activity. Some of pyrazine C—H and N—H acids also demonstrated antithrombotic and antiplatelet activity (Petrušewicz *et al.*, 1993).

Such pharmacological activity (in group CH– and NH– acids) is possibly the result of acid character of particle and their structure, as in case of well known inhibitors of cyclooxygenase (Petrušewicz *et al.*, 1993). Structural analysis of pyrazine-acetonitrile derivatives shows pyrazinyl-pyrazolidene tautomerism (Pilarski *et al.*, 1984) but crystal of 2-butyl 2-(3-chloropyrazin- (1*H*)-ylidene)-2-cyanoacetate appears as NH-acid.

In the molecule of the title compound (Fig. 1) the bond lengths and angles characterizing the geometry of the pyrazines skeleton are typical for this group compounds (Vishweshwar *et al.* 2000; Wardell *et al.* 2006). The compound is essentially planar except for the *n*-butoxy group (r.m.s. deviation from the least-squares plane - 0.0131 (1) Å for 11 non-H atoms. An intramolecular N2—H2B···O1 contact generates a S(6) ring motif which stabilizes the molecular conformation. The *n*-butoxy chain in the molecule is disordered over two sets of sites in a 0.50 (1):0.50 (1) ratio.

Experimental

2-butyl 2-(3-chloropyrazin-2(1*H*)-ylidene)-2-cyanoacetate was obtained by general method described in papers (Pilarski *et al.*, 1981; Pilarski *et al.*, 1982). Crystallization of this compound from methanol forms a crystal.

Refinement

Atoms O2, C8 (H8A, H8B), C9 (H9A, H9B), C10 (H10A, H10B), C11 (H11A, H11B, H11C) were disordered over two positions. During the refinement process the disordered atoms were refined with occupancies of 0.50 and 0.50. H atoms bonded to C were included in calculated positions and refined as riding on their parent C atom with C—H = 0.95 Å $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for aromatic, C—H = 0.99 Å $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for methylene and C—H = 0.98 Å $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ for methyl H atoms. The H2B atom was located from difference Fourier map and refined isotropically resulting in N—H bond length 0.87 (2) Å $U_{\text{iso}}(\text{H}) = 0.10 (2) \text{ \AA}^2$. The carbon atoms C8, C9, C10, C11 and C8A, C9A, C10A, C11A were located from a difference map, fixed at 1.50 for C—C distance and refined with the *DFIX* restraint. The Flack (1983) parameter was refined explicitly, with both *TWIN* and *BASF* parameters.

Figures

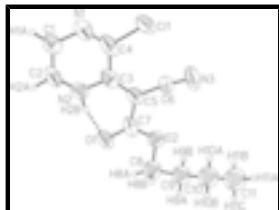


Fig. 1. The molecular structure of the title compound showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

n-Butyl 2-(3-chloro-1,2-dihydropyrazin-2-ylidene)-2-cyanoacetate

Crystal data

$C_{11}H_{12}ClN_3O_2$	$F_{000} = 528$
$M_r = 253.69$	$D_x = 1.27 \text{ Mg m}^{-3}$
Monoclinic, <i>Cc</i>	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: C -2yc	Cell parameters from 1500 reflections
$a = 4.918 (3) \text{ \AA}$	$\theta = 2.5\text{--}32.3^\circ$
$b = 25.642 (7) \text{ \AA}$	$\mu = 0.28 \text{ mm}^{-1}$
$c = 10.573 (4) \text{ \AA}$	$T = 120 \text{ K}$
$\beta = 95.80 (3)^\circ$	Block, yellow
$V = 1326.7 (9) \text{ \AA}^3$	$0.57 \times 0.11 \times 0.07 \text{ mm}$
$Z = 4$	

Data collection

Oxford Diffraction KM-4/Xcalibur diffractometer with a Sapphire2 (large Be window) detector	1687 independent reflections
Monochromator: graphite	1219 reflections with $I > 2\sigma(I)$
Detector resolution: $8.1883 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.034$
$T = 120 \text{ K}$	$\theta_{\text{max}} = 25.5^\circ$
0.75° wide ω scans	$\theta_{\text{min}} = 2.5^\circ$
Absorption correction: Gaussian (CrysAlis Pro; Oxford Diffraction, 2007)	$h = -3 \rightarrow 5$
$T_{\text{min}} = 0.923$, $T_{\text{max}} = 0.987$	$k = -31 \rightarrow 31$
4629 measured reflections	$l = -12 \rightarrow 12$

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
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.1833P)^2]$
$wR(F^2) = 0.156$	where $P = (F_o^2 + 2F_c^2)/3$
	$(\Delta/\sigma)_{\text{max}} < 0.001$

$S = 1.04$	$\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$
1687 reflections	$\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$
154 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 466 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.05 (18)
Secondary atom site location: difference Fourier map	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C11	0.7083 (3)	0.42260 (5)	0.30244 (15)	0.0753 (4)	
O1	0.0928 (8)	0.54438 (16)	0.6099 (3)	0.0731 (12)	
N1	0.4291 (11)	0.36488 (18)	0.4525 (5)	0.0827 (13)	
N2	0.1819 (9)	0.4445 (2)	0.5738 (4)	0.0612 (12)	
N3	0.7225 (16)	0.55178 (17)	0.2917 (6)	0.0874 (12)	
C1	0.2496 (17)	0.3549 (3)	0.5468 (7)	0.0905 (19)	
H1A	0.2102	0.3199	0.5681	0.109*	
C2	0.1303 (11)	0.3956 (3)	0.6086 (5)	0.0695 (16)	
H2A	0.0153	0.3889	0.6737	0.083*	
C3	0.3572 (10)	0.4596 (2)	0.4816 (4)	0.0548 (12)	
C4	0.4796 (11)	0.4144 (2)	0.4225 (4)	0.0649 (13)	
C5	0.4002 (10)	0.5136 (2)	0.4565 (4)	0.0569 (10)	
C6	0.5828 (11)	0.5330 (2)	0.3632 (5)	0.0617 (11)	
C7	0.2549 (12)	0.5528 (2)	0.5259 (5)	0.0626 (15)	
O2	0.3471 (16)	0.6051 (3)	0.5012 (7)	0.050 (2)*	0.5
C8	0.202 (2)	0.6474 (4)	0.5635 (11)	0.056 (3)*	0.5
H8A	0.2504	0.647	0.6566	0.067*	0.5
H8B	0.0014	0.6434	0.5458	0.067*	0.5
C9	0.296 (2)	0.6977 (4)	0.5064 (9)	0.070 (3)*	0.5
H9A	0.4939	0.7017	0.5331	0.084*	0.5
H9B	0.2014	0.7269	0.5444	0.084*	0.5
C10	0.253 (3)	0.7037 (4)	0.3607 (9)	0.072 (3)*	0.5
H10A	0.3655	0.6769	0.3231	0.086*	0.5
H10B	0.0594	0.6955	0.3331	0.086*	0.5
C11	0.316 (3)	0.7546 (5)	0.3052 (16)	0.095 (4)*	0.5

supplementary materials

H11A	0.1591	0.7664	0.248	0.143*	0.5
H11B	0.4758	0.751	0.2573	0.143*	0.5
H11C	0.3558	0.7802	0.3734	0.143*	0.5
O2A	0.268 (2)	0.6013 (4)	0.4705 (9)	0.071 (3)*	0.5
C8A	0.111 (3)	0.6434 (5)	0.5272 (13)	0.080 (4)*	0.5
H8AA	0.1828	0.6493	0.6169	0.095*	0.5
H8AB	-0.0843	0.6336	0.5246	0.095*	0.5
C9A	0.142 (3)	0.6924 (5)	0.4496 (14)	0.102 (4)*	0.5
H9A1	0.0102	0.6892	0.3728	0.122*	0.5
H9A2	0.0775	0.7217	0.4998	0.122*	0.5
C10A	0.402 (3)	0.7092 (5)	0.4057 (13)	0.092 (3)*	0.5
H10C	0.4668	0.6798	0.3559	0.11*	0.5
H10D	0.5335	0.7124	0.4827	0.11*	0.5
C11A	0.433 (4)	0.7571 (5)	0.3292 (13)	0.089 (4)*	0.5
H11D	0.6227	0.7691	0.3421	0.133*	0.5
H11E	0.3116	0.7843	0.3561	0.133*	0.5
H11F	0.3845	0.7493	0.239	0.133*	0.5
H2B	0.150 (14)	0.4691 (19)	0.627 (5)	0.10 (2)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0730 (7)	0.0881 (7)	0.0692 (6)	0.0104 (9)	0.0279 (5)	-0.0026 (8)
O1	0.085 (3)	0.067 (2)	0.073 (2)	0.003 (2)	0.035 (2)	0.0011 (18)
N1	0.098 (3)	0.070 (3)	0.085 (3)	0.007 (2)	0.036 (2)	0.001 (2)
N2	0.063 (3)	0.067 (3)	0.055 (2)	0.006 (2)	0.013 (2)	-0.003 (2)
N3	0.087 (3)	0.098 (3)	0.082 (3)	-0.002 (3)	0.034 (2)	0.021 (3)
C1	0.119 (5)	0.063 (3)	0.097 (4)	0.004 (3)	0.049 (4)	-0.001 (3)
C2	0.075 (4)	0.071 (4)	0.067 (3)	-0.004 (3)	0.028 (3)	0.002 (3)
C3	0.049 (3)	0.073 (3)	0.042 (2)	0.003 (2)	0.0044 (19)	-0.007 (2)
C4	0.063 (3)	0.080 (4)	0.053 (2)	0.009 (2)	0.014 (2)	-0.002 (2)
C5	0.055 (2)	0.065 (3)	0.052 (2)	-0.002 (2)	0.0109 (18)	0.0014 (17)
C6	0.058 (2)	0.073 (3)	0.056 (2)	0.002 (2)	0.014 (2)	0.002 (2)
C7	0.069 (3)	0.060 (4)	0.062 (3)	-0.007 (3)	0.018 (3)	0.004 (3)

Geometric parameters (\AA , $^\circ$)

Cl1—C4	1.791 (5)	C9—H9A	0.99
O1—C7	1.271 (7)	C9—H9B	0.99
N1—C4	1.338 (7)	C10—C11	1.478 (14)
N1—C1	1.421 (8)	C10—H10A	0.99
N2—C2	1.338 (9)	C10—H10B	0.99
N2—C3	1.419 (8)	C11—H11A	0.98
N2—H2B	0.87 (2)	C11—H11B	0.98
N3—C6	1.175 (8)	C11—H11C	0.98
C1—C2	1.392 (10)	O2A—C8A	1.489 (17)
C1—H1A	0.95	C8A—C9A	1.516 (14)
C2—H2A	0.95	C8A—H8AA	0.99
C3—C5	1.428 (7)	C8A—H8AB	0.99

C3—C4	1.475 (7)	C9A—C10A	1.469 (14)
C5—C7	1.472 (8)	C9A—H9A1	0.99
C5—C6	1.486 (7)	C9A—H9A2	0.99
C7—O2A	1.379 (11)	C10A—C11A	1.487 (14)
C7—O2	1.448 (10)	C10A—H10C	0.99
O2—C8	1.489 (13)	C10A—H10D	0.99
C8—C9	1.514 (12)	C11A—H11D	0.98
C8—H8A	0.99	C11A—H11E	0.98
C8—H8B	0.99	C11A—H11F	0.98
C9—C10	1.541 (12)		
C4—N1—C1	118.8 (5)	C10—C9—H9A	107.8
C2—N2—C3	126.2 (5)	C8—C9—H9B	107.8
C2—N2—H2B	117 (5)	C10—C9—H9B	107.8
C3—N2—H2B	114 (5)	H9A—C9—H9B	107.2
C2—C1—N1	121.0 (6)	C11—C10—C9	118.2 (10)
C2—C1—H1A	119.5	C11—C10—H10A	107.8
N1—C1—H1A	119.5	C9—C10—H10A	107.8
N2—C2—C1	118.3 (5)	C11—C10—H10B	107.8
N2—C2—H2A	120.9	C9—C10—H10B	107.8
C1—C2—H2A	120.9	H10A—C10—H10B	107.1
N2—C3—C5	120.3 (5)	C7—O2A—C8A	115.7 (8)
N2—C3—C4	112.3 (5)	O2A—C8A—C9A	107.3 (11)
C5—C3—C4	127.5 (5)	O2A—C8A—H8AA	110.2
N1—C4—C3	123.5 (4)	C9A—C8A—H8AA	110.2
N1—C4—C11	115.1 (4)	O2A—C8A—H8AB	110.2
C3—C4—C11	121.4 (4)	C9A—C8A—H8AB	110.2
C3—C5—C7	118.7 (4)	H8AA—C8A—H8AB	108.5
C3—C5—C6	124.0 (4)	C10A—C9A—C8A	123.5 (13)
C7—C5—C6	117.3 (5)	C10A—C9A—H9A1	106.5
N3—C6—C5	175.5 (5)	C8A—C9A—H9A1	106.5
O1—C7—O2A	120.7 (6)	C10A—C9A—H9A2	106.5
O1—C7—O2	120.9 (5)	C8A—C9A—H9A2	106.5
O2A—C7—O2	19.8 (5)	H9A1—C9A—H9A2	106.5
O1—C7—C5	127.1 (5)	C9A—C10A—C11A	123.6 (13)
O2A—C7—C5	111.0 (6)	C9A—C10A—H10C	106.4
O2—C7—C5	111.5 (5)	C11A—C10A—H10C	106.4
C7—O2—C8	115.0 (7)	C9A—C10A—H10D	106.4
O2—C8—C9	105.3 (8)	C11A—C10A—H10D	106.4
O2—C8—H8A	110.7	H10C—C10A—H10D	106.5
C9—C8—H8A	110.7	C10A—C11A—H11D	109.5
O2—C8—H8B	110.7	C10A—C11A—H11E	109.5
C9—C8—H8B	110.7	H11D—C11A—H11E	109.5
H8A—C8—H8B	108.8	C10A—C11A—H11F	109.5
C8—C9—C10	117.8 (9)	H11D—C11A—H11F	109.5
C8—C9—H9A	107.8	H11E—C11A—H11F	109.5
C4—N1—C1—C2	-0.9 (10)	C6—C5—C7—O1	-179.2 (5)
C3—N2—C2—C1	-2.4 (9)	C3—C5—C7—O2A	-166.0 (6)
N1—C1—C2—N2	2.2 (11)	C6—C5—C7—O2A	13.6 (8)

supplementary materials

C2—N2—C3—C5	-178.1 (5)	C3—C5—C7—O2	172.8 (5)
C2—N2—C3—C4	1.2 (7)	C6—C5—C7—O2	-7.6 (8)
C1—N1—C4—C3	-0.4 (8)	O1—C7—O2—C8	-10.3 (11)
C1—N1—C4—C11	-179.9 (5)	O2A—C7—O2—C8	85.0 (19)
N2—C3—C4—N1	0.3 (7)	C5—C7—O2—C8	177.5 (7)
C5—C3—C4—N1	179.5 (5)	C7—O2—C8—C9	-170.4 (8)
N2—C3—C4—C11	179.8 (3)	O2—C8—C9—C10	56.8 (12)
C5—C3—C4—C11	-1.0 (7)	C8—C9—C10—C11	173.4 (12)
N2—C3—C5—C7	-1.4 (6)	O1—C7—O2A—C8A	7.6 (13)
C4—C3—C5—C7	179.5 (5)	O2—C7—O2A—C8A	-89.0 (19)
N2—C3—C5—C6	179.1 (5)	C5—C7—O2A—C8A	175.8 (9)
C4—C3—C5—C6	-0.1 (8)	C7—O2A—C8A—C9A	-177.5 (10)
C3—C5—C6—N3	18E1(10)	O2A—C8A—C9A—C10A	-42.8 (19)
C7—C5—C6—N3	0(8)	C8A—C9A—C10A—C11A	179.8 (14)
C3—C5—C7—O1	1.2 (8)		

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2B \cdots O1	0.87 (2)	1.96 (5)	2.632 (6)	133 (6)

Fig. 1

