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(*E*)-(4-Bromobenzylidene)amino cyclopropanecarboxylate

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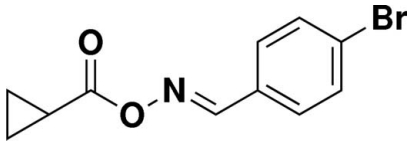
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.082; data-to-parameter ratio = 13.7.

In the title compound, $C_{11}H_{10}BrNO_2$, the dihedral angle between the benzene and cyclopropane ring planes is 49.4 (3)°. The C—C—N—O torsion angle is −175.1 (3)°, which indicates that the C=N double bond is in the *E* configuration.

Related literature

For details of the synthesis, see: Liu *et al.* (2011*a*). For the KARI (ketol–acid reductoisomerase) activity of related compounds, see: Liu *et al.* (2009*a*,*b*, 2010, 2011*b*,*c*,*d*). For related structures, see: Liu *et al.* (2011*a*,*c*).



Experimental

Crystal data

$C_{11}H_{10}BrNO_2$
M_r = 268.11
Monoclinic, $P2_1/c$
a = 13.209 (3) Å
b = 13.789 (3) Å
c = 5.8714 (12) Å
β = 98.27 (3)°
V = 1058.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.86 mm^{-1}
T = 113 K
0.16 × 0.14 × 0.12 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.577, T_{max} = 0.654
5989 measured reflections
1862 independent reflections
1320 reflections with $I > 2\sigma(I)$
R_{int} = 0.096

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.082
S = 0.96
1862 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

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: DS2156).

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supporting information

Acta Cryst. (2012). E**68**, o493 [doi:10.1107/S1600536812002048]

(*E*)-(4-Bromobenzylidene)amino cyclopropanecarboxylate

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S1. Experimental

To a solution of 4-bromobenzaldehyde oxime (7.50 mmol in 25 ml THF) and 7.5 mmol Et3N, was added the cyclopropanecarbonyl chloride. Then the mixture was vigorously stirred at room temperature for overnight. The corresponding product precipitated immediately. Compound was dissolved in hot alcohol and the resulting solution was allowed to stand in air at room temperature to give single crystal.

S2. 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).

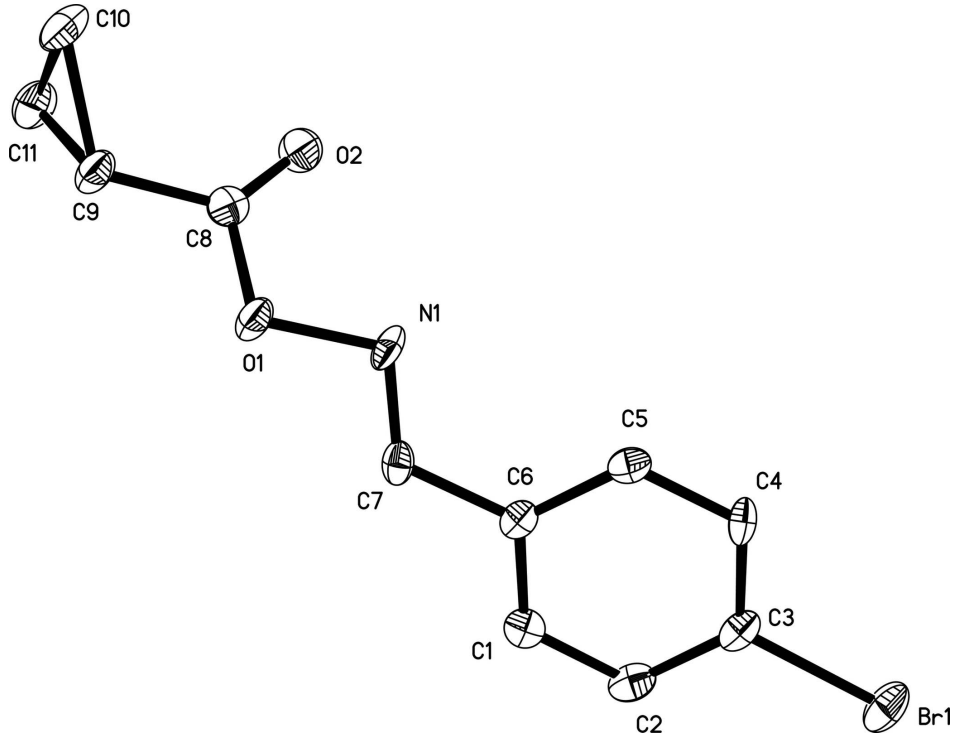

Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

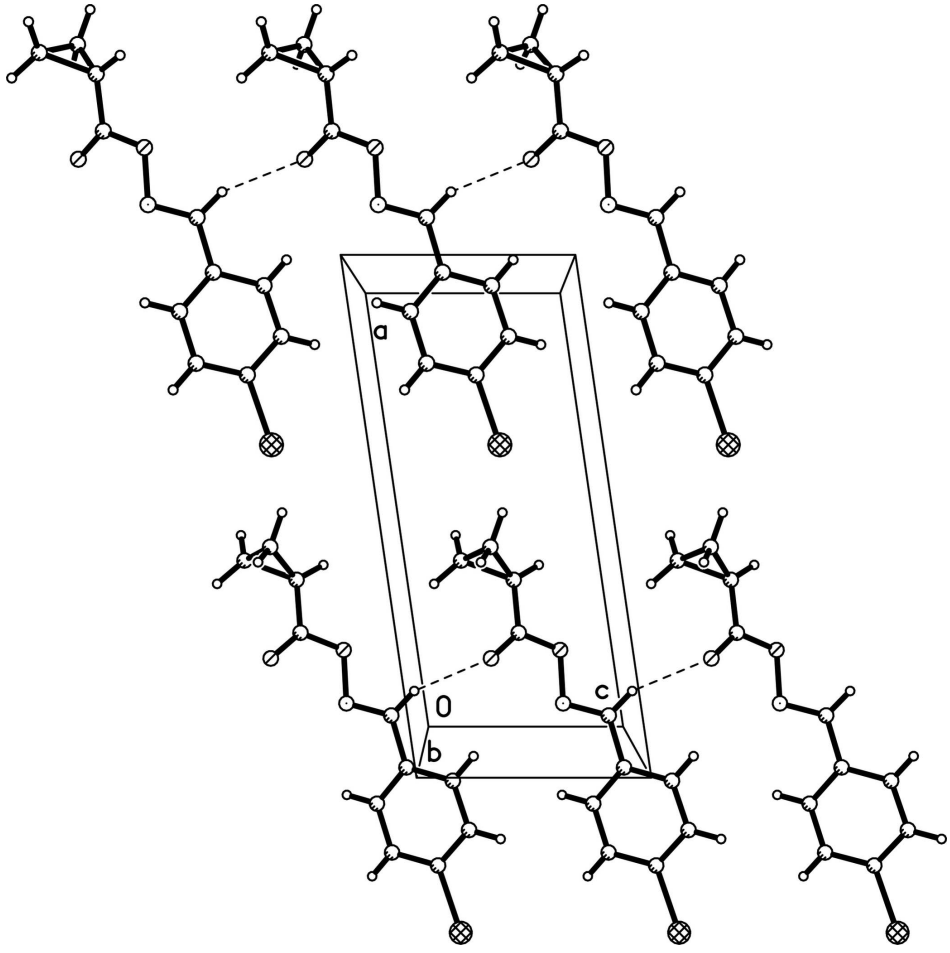

Figure 2

The crystal packing for (I).

(*E*)-(4-Bromobenzylidene)amino cyclopropanecarboxylate

Crystal data

$C_{11}H_{10}BrNO_2$
$M_r = 268.11$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.209$ (3) Å
$b = 13.789$ (3) Å
$c = 5.8714$ (12) Å
$\beta = 98.27$ (3)°
$V = 1058.3$ (4) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.683$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2894 reflections
$\theta = 2.2$–27.5°
$\mu = 3.86$ mm^{-1}
$T = 113$ K
Prism, colorless
0.16 × 0.14 × 0.12 mm

Data collection

Rigaku Saturn diffractometer
Radiation source: rotating anode
Confocal monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.577$, $T_{max} = 0.654$
5989 measured reflections
1862 independent reflections
1320 reflections with $I > 2\sigma(I)$

R_{int} = 0.096
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −15→14
k = −15→16
l = −6→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.082
S = 0.96
1862 reflections
136 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
$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 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}
Br1	0.63851 (3)	0.63645 (3)	1.06308 (6)	0.02820 (17)
O1	1.21657 (17)	0.58865 (18)	0.7082 (4)	0.0204 (6)
O2	1.20566 (19)	0.68074 (19)	0.3851 (4)	0.0246 (6)
N1	1.1064 (2)	0.5958 (2)	0.6861 (5)	0.0207 (7)
C1	0.9529 (3)	0.6535 (2)	1.1289 (6)	0.0183 (9)
H1	1.0055	0.6740	1.2410	0.022*
C2	0.8530 (3)	0.6600 (2)	1.1709 (6)	0.0206 (9)
H2	0.8381	0.6849	1.3094	0.025*
C3	0.7756 (3)	0.6286 (2)	1.0033 (6)	0.0181 (9)
C4	0.7967 (3)	0.5906 (3)	0.7961 (6)	0.0167 (8)
H4	0.7441	0.5693	0.6849	0.020*
C5	0.8972 (3)	0.5849 (3)	0.7583 (6)	0.0177 (8)
H5	0.9122	0.5592	0.6205	0.021*
C6	0.9762 (3)	0.6170 (2)	0.9223 (6)	0.0160 (8)
C7	1.0830 (3)	0.6136 (2)	0.8868 (6)	0.0164 (8)
H7	1.1344	0.6243	1.0100	0.020*
C8	1.2549 (3)	0.6312 (3)	0.5280 (6)	0.0187 (9)
C9	1.3629 (3)	0.6058 (3)	0.5407 (6)	0.0215 (9)
H9	1.3922	0.5636	0.6676	0.026*
C10	1.4024 (3)	0.5931 (3)	0.3108 (6)	0.0291 (10)
H10A	1.4536	0.5436	0.3005	0.035*
H10B	1.3543	0.6027	0.1714	0.035*

C11	1.4328 (3)	0.6793 (3)	0.4557 (6)	0.0287 (10)
H11A	1.4036	0.7414	0.4038	0.034*
H11B	1.5028	0.6823	0.5328	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0195 (3)	0.0277 (3)	0.0407 (3)	0.00510 (17)	0.0154 (2)	0.00313 (19)
O1	0.0144 (14)	0.0227 (16)	0.0259 (14)	0.0002 (12)	0.0085 (11)	0.0042 (12)
O2	0.0247 (16)	0.0239 (16)	0.0252 (14)	0.0030 (13)	0.0040 (12)	0.0030 (12)
N1	0.0111 (17)	0.026 (2)	0.0274 (17)	0.0028 (14)	0.0087 (14)	−0.0021 (15)
C1	0.022 (2)	0.012 (2)	0.0204 (19)	0.0001 (16)	0.0028 (16)	0.0003 (15)
C2	0.026 (2)	0.015 (2)	0.0227 (19)	0.0055 (17)	0.0118 (17)	−0.0024 (16)
C3	0.019 (2)	0.011 (2)	0.026 (2)	0.0020 (16)	0.0096 (17)	0.0032 (16)
C4	0.0088 (19)	0.013 (2)	0.028 (2)	0.0003 (16)	0.0012 (15)	−0.0015 (17)
C5	0.021 (2)	0.016 (2)	0.0172 (18)	0.0015 (17)	0.0063 (16)	0.0006 (16)
C6	0.017 (2)	0.012 (2)	0.0206 (19)	0.0013 (15)	0.0054 (16)	0.0020 (15)
C7	0.012 (2)	0.012 (2)	0.025 (2)	0.0015 (15)	0.0013 (16)	0.0026 (15)
C8	0.020 (2)	0.016 (2)	0.0197 (19)	−0.0078 (16)	0.0029 (17)	−0.0065 (17)
C9	0.017 (2)	0.024 (2)	0.0259 (19)	0.0019 (18)	0.0098 (16)	0.0054 (17)
C10	0.023 (2)	0.035 (3)	0.032 (2)	0.001 (2)	0.0157 (18)	−0.004 (2)
C11	0.020 (2)	0.036 (3)	0.032 (2)	−0.009 (2)	0.0099 (18)	0.002 (2)

Geometric parameters (Å, º)

Br1—C3	1.896 (4)	C5—C6	1.386 (5)
O1—C8	1.369 (4)	C5—H5	0.9300
O1—N1	1.445 (3)	C6—C7	1.456 (5)
O2—C8	1.199 (4)	C7—H7	0.9300
N1—C7	1.285 (4)	C8—C9	1.460 (5)
C1—C2	1.379 (5)	C9—C11	1.504 (5)
C1—C6	1.389 (5)	C9—C10	1.525 (5)
C1—H1	0.9300	C9—H9	0.9800
C2—C3	1.383 (5)	C10—C11	1.483 (5)
C2—H2	0.9300	C10—H10A	0.9700
C3—C4	1.390 (5)	C10—H10B	0.9700
C4—C5	1.379 (4)	C11—H11A	0.9700
C4—H4	0.9300	C11—H11B	0.9700
C8—O1—N1	112.4 (3)	C6—C7—H7	119.9
C7—N1—O1	107.6 (3)	O2—C8—O1	124.1 (3)
C2—C1—C6	121.2 (3)	O2—C8—C9	126.9 (3)
C2—C1—H1	119.4	O1—C8—C9	109.0 (3)
C6—C1—H1	119.4	C8—C9—C11	117.6 (3)
C1—C2—C3	118.8 (3)	C8—C9—C10	116.0 (3)
C1—C2—H2	120.6	C11—C9—C10	58.6 (2)
C3—C2—H2	120.6	C8—C9—H9	117.2
C2—C3—C4	121.3 (3)	C11—C9—H9	117.2

C2—C3—Br1	118.6 (3)	C10—C9—H9	117.2
C4—C3—Br1	120.1 (3)	C11—C10—C9	60.0 (2)
C5—C4—C3	118.8 (3)	C11—C10—H10A	117.8
C5—C4—H4	120.6	C9—C10—H10A	117.8
C3—C4—H4	120.6	C11—C10—H10B	117.8
C4—C5—C6	121.0 (3)	C9—C10—H10B	117.8
C4—C5—H5	119.5	H10A—C10—H10B	114.9
C6—C5—H5	119.5	C10—C11—C9	61.4 (2)
C5—C6—C1	118.9 (3)	C10—C11—H11A	117.6
C5—C6—C7	122.6 (3)	C9—C11—H11A	117.6
C1—C6—C7	118.5 (3)	C10—C11—H11B	117.6
N1—C7—C6	120.2 (3)	C9—C11—H11B	117.6
N1—C7—H7	119.9	H11A—C11—H11B	114.7

C8—O1—N1—C7	−140.2 (3)	O1—N1—C7—C6	−175.1 (3)
C6—C1—C2—C3	0.5 (5)	C5—C6—C7—N1	11.9 (5)
C1—C2—C3—C4	0.4 (5)	C1—C6—C7—N1	−168.3 (3)
C1—C2—C3—Br1	179.4 (3)	N1—O1—C8—O2	10.1 (5)
C2—C3—C4—C5	−0.4 (5)	N1—O1—C8—C9	−169.7 (3)
Br1—C3—C4—C5	−179.4 (3)	O2—C8—C9—C11	32.6 (5)
C3—C4—C5—C6	−0.4 (5)	O1—C8—C9—C11	−147.6 (3)
C4—C5—C6—C1	1.2 (5)	O2—C8—C9—C10	−33.9 (5)
C4—C5—C6—C7	−179.0 (3)	O1—C8—C9—C10	145.9 (3)
C2—C1—C6—C5	−1.2 (5)	C8—C9—C10—C11	107.8 (4)
C2—C1—C6—C7	179.0 (3)	C8—C9—C11—C10	−105.1 (4)