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3-[Chloro(phenyl)methyl]-6-methyl-1,2-benzoxazole

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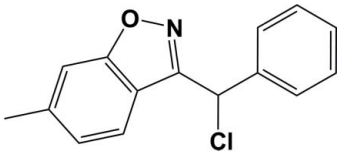
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.125; data-to-parameter ratio = 12.8.

The title compound, $C_{15}H_{12}ClNO$, is a functionalized 1,2-benzoxazole with a chloro(phenyl)methyl substituent. The molecule is V-shaped, the dihedral angle between the mean plane of the 1,2-benzoxazole system [maximum deviation = 0.023 (3) Å for the N atom] and the phenyl ring being 70.33 (14)°. There are no hydrogen-bonding interactions in the crystal structure, which is stabilized by van der Waals interactions only.

Related literature

For the synthesis of the title compound, see: Veerareddy *et al.* (2011). For related structures, see: Atovmyan & Aliev (1994); Hu *et al.* (2009); Korlyukov *et al.* (2003).



Experimental

Crystal data

$C_{15}H_{12}ClNO$ M_r = 257.71
Monoclinic, $P2_1/c$
a = 13.2075 (8) Å
b = 6.5888 (4) Å
c = 15.1224 (8) Å
β = 103.738 (3)°
V = 1278.33 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 293 K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.919, T_{max} = 0.945
10507 measured reflections
2087 independent reflections
1621 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.125
S = 1.06
2087 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2326).

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supporting information

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3-[Chloro(phenyl)methyl]-6-methyl-1,2-benzoxazole

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S1. Comment

Benzisoxazole is an aromatic organic compound with a molecular formula C_7H_5NO containing a benzene-fused isoxazole ring structure. Benzisoxazole is primarily used in industry and research. Being a heterocyclic compound, benzisoxazole finds use in research as a starting material for the synthesis of larger, usually bioactive structures. Isoxazole and benzisoxazole are important classes of nitrogen-oxygen containing heterocycles. They have extensive applications as structural units of various biologically important molecules and as useful intermediates in medicinal chemistry. Among them, 3–substituted–1,2–benzisoxazole and their derivatives are emerging as potential antipsychotic compounds. For example, 1,2–benzisoxazole–3–methanesulfonamide, also known as zonisamide, is an efficient antiseizure agent. It has been reported that it blocks the repetitive firing of voltage–sensitive sodium channels and reduces voltage–sensitive T–type calcium currents (Veerareddy *et al.*, 2011).

In molecular structure of the title functionalized 1,2-benzoxazole compound, (I), is illustrated in Fig. 1. The bond length and angles are in agreement with those found for closely related structures, for example, 6-tert-butyl-4,5-dichloro-3-ethyl-4,5-dihydro-2,1-benzoisoxazole (II) [Atovmyan & Aliev, 1994], 3-(1,3-dioxolan-2-yl)-4,6-dinitrobenzo[d]isoxazole (III) [Korlyukov *et al.*, 2003], and N-Phenyl-4-(8-phenyl-4,5-dihydro-1,2-benzoxazolo- [4,5-d]thiazol-2-yl)-piperidine-1-carboxamide (IV) [Hu *et al.*, 2009]. The widening of the exocyclic angle C10—C9—C3 [113.4 (2)°] from the normal value of 109° may be due to repulsion between neighbouring H atoms [H9··· H11 = 2.2495 (1) Å]. The exocyclic angles C9—C3—C3a [132.1 (2)°] and C3—C3a—C4 [138.2 (2)°] deviate significantly from the normal value of 120° and this may be due to the intramolecular non-bonded interactions between the chlorine atom and H-atom H4 at C10 [Cl··· H4 = 3.1169 (7) Å]. The isoxazole ring (O1,N2,C3,C3a,C7a) is planar [max. deviation 0.007 (3) Å], with the chloro(phenyl)-methyl substituent being nearly normal to the plane of the five membered ring [N2-C3-C9-C10 = 100.1 (3)°], similar to the situation in compound (II) (Atovmyan & Aliev, 1994). The dihedral angle between the mean plane of the 1,2-benzoxazole [max. deviation 0.023 (3) Å] and the phenyl ring (C10-C15) is 70.33 (14)°.

Crystal packing of compound (I) is illustrated in Fig. 2. There are no significant non-bonded interactions present and the crystal structure is stabilized by van der Waals interactions only.

S2. Experimental

The compound was synthesized following the published procedure (Veerareddy *et al.*, 2011).

S3. Refinement

All the H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H = 0.93Å (aromatic), 0.98Å (methine) and 0.96Å (methyl), and refined using a riding model with U_{iso}(H)= 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

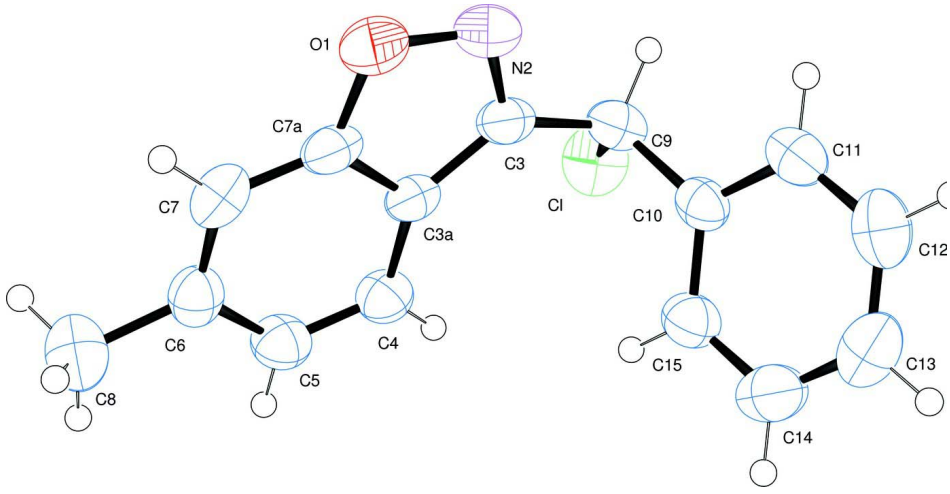

Figure 1

The molecular structure of compound (I), showing the numbering sheme and displacement ellipsoids drawn at the 50% probability level.

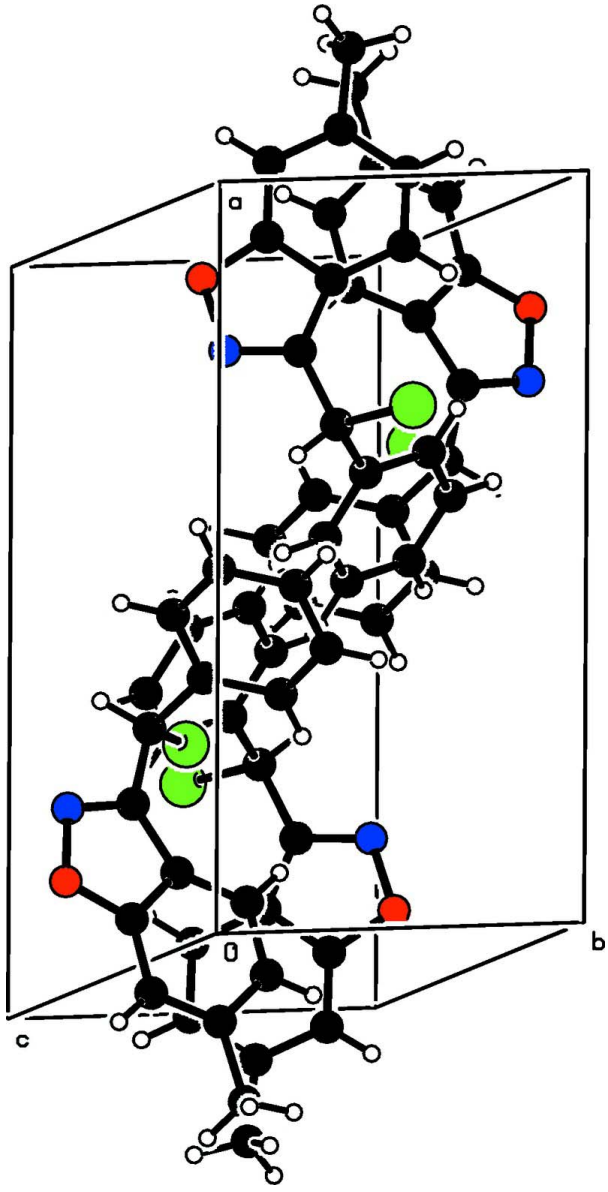

Figure 2

A view of the crystal packing of compound (I).

3-[Chloro(phenyl)methyl]-6-methyl-1,2-benzoxazole

Crystal data

$C_{15}H_{12}ClNO$
$M_r = 257.71$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.2075\ (8)$ Å
$b = 6.5888\ (4)$ Å
$c = 15.1224\ (8)$ Å
$\beta = 103.738\ (3)°$
$V = 1278.33\ (13)$ Å^3
$Z = 4$

$F(000) = 536$
$D_x = 1.339$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 20–30°$
$\mu = 0.29$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.919, T_{max} = 0.945
10507 measured reflections
2087 independent reflections
1621 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 24.4°, θ_{min} = 2.8°
h = −15→15
k = −5→7
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.125
S = 1.06
2087 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.7285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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}
C14	0.3858 (2)	0.3538 (4)	0.10340 (19)	0.0625 (7)
H14	0.3663	0.4825	0.0803	0.075*
C15	0.33247 (19)	0.2630 (4)	0.16026 (17)	0.0514 (6)
H15	0.2771	0.3303	0.1756	0.062*
C10	0.36083 (17)	0.0718 (3)	0.19482 (15)	0.0426 (6)
C11	0.44364 (18)	−0.0247 (4)	0.17192 (16)	0.0512 (6)
H11	0.4639	−0.1530	0.1953	0.061*
C12	0.4965 (2)	0.0676 (5)	0.11477 (18)	0.0614 (7)
H12	0.5521	0.0012	0.0995	0.074*
C13	0.4678 (2)	0.2562 (5)	0.08037 (18)	0.0637 (8)
H13	0.5035	0.3181	0.0416	0.076*
C9	0.30211 (18)	−0.0408 (4)	0.25392 (16)	0.0499 (6)
H9	0.3434	−0.1605	0.2783	0.060*
C3	0.19728 (18)	−0.1135 (3)	0.20317 (16)	0.0453 (6)
C3A	0.10029 (17)	−0.0106 (3)	0.17045 (15)	0.0407 (5)
C4	0.05889 (18)	0.1827 (4)	0.17530 (16)	0.0474 (6)

H4	0.0998	0.2874	0.2060	0.057*
C5	−0.04334 (19)	0.2133 (4)	0.13360 (17)	0.0512 (6)
H5	−0.0716	0.3417	0.1366	0.061*
C6	−0.10804 (18)	0.0600 (4)	0.08627 (16)	0.0486 (6)
C7	−0.06762 (19)	−0.1303 (4)	0.08068 (17)	0.0526 (6)
H7	−0.1082	−0.2348	0.0494	0.063*
C7A	0.03587 (19)	−0.1596 (3)	0.12364 (17)	0.0476 (6)
C8	−0.2204 (2)	0.1048 (5)	0.0429 (2)	0.0708 (8)
H8A	−0.2352	0.2441	0.0536	0.106*
H8B	−0.2642	0.0181	0.0687	0.106*
H8C	−0.2336	0.0809	−0.0215	0.106*
N2	0.19137 (18)	−0.3037 (3)	0.17984 (18)	0.0657 (6)
O1	0.08903 (15)	−0.3377 (3)	0.12767 (15)	0.0693 (6)
Cl	0.28938 (6)	0.11252 (13)	0.34931 (5)	0.0704 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C14	0.0699 (18)	0.0508 (17)	0.0611 (16)	−0.0066 (14)	0.0044 (14)	0.0094 (13)
C15	0.0511 (14)	0.0432 (15)	0.0587 (15)	0.0055 (11)	0.0106 (11)	0.0002 (12)
C10	0.0392 (12)	0.0423 (14)	0.0416 (12)	0.0019 (10)	0.0006 (9)	−0.0024 (10)
C11	0.0486 (14)	0.0475 (15)	0.0531 (14)	0.0081 (12)	0.0031 (11)	−0.0021 (12)
C12	0.0488 (15)	0.079 (2)	0.0567 (16)	0.0005 (14)	0.0144 (12)	−0.0122 (15)
C13	0.0619 (17)	0.078 (2)	0.0519 (15)	−0.0193 (15)	0.0139 (13)	0.0000 (15)
C9	0.0551 (15)	0.0430 (14)	0.0513 (14)	0.0105 (11)	0.0120 (11)	0.0057 (11)
C3	0.0534 (14)	0.0350 (13)	0.0504 (13)	0.0023 (10)	0.0179 (11)	0.0070 (10)
C3A	0.0484 (13)	0.0326 (12)	0.0441 (12)	−0.0027 (10)	0.0169 (10)	0.0027 (10)
C4	0.0526 (14)	0.0376 (14)	0.0511 (14)	−0.0020 (11)	0.0103 (11)	−0.0060 (11)
C5	0.0556 (15)	0.0424 (15)	0.0569 (14)	0.0056 (12)	0.0158 (12)	−0.0026 (12)
C6	0.0458 (13)	0.0564 (17)	0.0450 (13)	−0.0035 (12)	0.0137 (10)	0.0013 (11)
C7	0.0540 (15)	0.0498 (16)	0.0560 (15)	−0.0153 (12)	0.0173 (12)	−0.0054 (12)
C7A	0.0579 (15)	0.0313 (13)	0.0572 (14)	−0.0044 (11)	0.0207 (12)	0.0029 (11)
C8	0.0540 (16)	0.080 (2)	0.0760 (19)	−0.0010 (14)	0.0105 (14)	−0.0066 (16)
N2	0.0642 (15)	0.0356 (13)	0.0970 (18)	0.0053 (10)	0.0186 (13)	0.0041 (12)
O1	0.0672 (12)	0.0324 (10)	0.1063 (16)	−0.0036 (9)	0.0168 (11)	−0.0070 (10)
Cl	0.0770 (5)	0.0849 (6)	0.0506 (4)	−0.0038 (4)	0.0177 (3)	−0.0093 (3)

Geometric parameters (Å, º)

C14—C15	1.371 (4)	C3—C3A	1.430 (3)
C14—C13	1.374 (4)	C3A—C7A	1.380 (3)
C14—H14	0.9300	C3A—C4	1.395 (3)
C15—C10	1.381 (3)	C4—C5	1.363 (3)
C15—H15	0.9300	C4—H4	0.9300
C10—C11	1.378 (3)	C5—C6	1.404 (4)
C10—C9	1.510 (3)	C5—H5	0.9300
C11—C12	1.375 (4)	C6—C7	1.374 (4)
C11—H11	0.9300	C6—C8	1.502 (4)

C12—C13	1.365 (4)	C7—C7A	1.380 (3)
C12—H12	0.9300	C7—H7	0.9300
C13—H13	0.9300	C7A—O1	1.361 (3)
C9—C3	1.494 (3)	C8—H8A	0.9600
C9—Cl	1.801 (2)	C8—H8B	0.9600
C9—H9	0.9800	C8—H8C	0.9600
C3—N2	1.299 (3)	N2—O1	1.412 (3)

C15—C14—C13	120.5 (3)	C7A—C3A—C4	118.4 (2)
C15—C14—H14	119.7	C7A—C3A—C3	103.5 (2)
C13—C14—H14	119.7	C4—C3A—C3	138.2 (2)
C14—C15—C10	120.1 (2)	C5—C4—C3A	118.0 (2)
C14—C15—H15	119.9	C5—C4—H4	121.0
C10—C15—H15	119.9	C3A—C4—H4	121.0
C11—C10—C15	119.1 (2)	C4—C5—C6	123.0 (2)
C11—C10—C9	118.2 (2)	C4—C5—H5	118.5
C15—C10—C9	122.7 (2)	C6—C5—H5	118.5
C12—C11—C10	120.3 (3)	C7—C6—C5	119.3 (2)
C12—C11—H11	119.8	C7—C6—C8	120.7 (2)
C10—C11—H11	119.8	C5—C6—C8	120.0 (2)
C13—C12—C11	120.4 (2)	C6—C7—C7A	117.0 (2)
C13—C12—H12	119.8	C6—C7—H7	121.5
C11—C12—H12	119.8	C7A—C7—H7	121.5
C12—C13—C14	119.6 (3)	O1—C7A—C3A	110.0 (2)
C12—C13—H13	120.2	O1—C7A—C7	125.8 (2)
C14—C13—H13	120.2	C3A—C7A—C7	124.3 (2)
C3—C9—C10	113.4 (2)	C6—C8—H8A	109.5
C3—C9—Cl	109.88 (16)	C6—C8—H8B	109.5
C10—C9—Cl	110.95 (17)	H8A—C8—H8B	109.5
C3—C9—H9	107.5	C6—C8—H8C	109.5
C10—C9—H9	107.5	H8A—C8—H8C	109.5
Cl—C9—H9	107.5	H8B—C8—H8C	109.5
N2—C3—C3A	111.9 (2)	C3—N2—O1	107.0 (2)
N2—C3—C9	116.0 (2)	C7A—O1—N2	107.68 (18)
C3A—C3—C9	132.1 (2)		

C13—C14—C15—C10	−0.1 (4)	C9—C3—C3A—C4	−5.6 (5)
C14—C15—C10—C11	0.5 (4)	C7A—C3A—C4—C5	0.2 (3)
C14—C15—C10—C9	−176.9 (2)	C3—C3A—C4—C5	−178.3 (2)
C15—C10—C11—C12	−0.6 (3)	C3A—C4—C5—C6	−0.1 (4)
C9—C10—C11—C12	176.9 (2)	C4—C5—C6—C7	−0.3 (4)
C10—C11—C12—C13	0.3 (4)	C4—C5—C6—C8	179.3 (2)
C11—C12—C13—C14	0.2 (4)	C5—C6—C7—C7A	0.6 (3)
C15—C14—C13—C12	−0.3 (4)	C8—C6—C7—C7A	−179.0 (2)
C11—C10—C9—C3	−106.5 (2)	C4—C3A—C7A—O1	−178.9 (2)
C15—C10—C9—C3	71.0 (3)	C3—C3A—C7A—O1	0.1 (3)
C11—C10—C9—Cl	129.31 (19)	C4—C3A—C7A—C7	0.2 (4)
C15—C10—C9—Cl	−53.2 (3)	C3—C3A—C7A—C7	179.1 (2)

C10—C9—C3—N2	100.1 (3)	C6—C7—C7A—O1	178.3 (2)
Cl—C9—C3—N2	−135.1 (2)	C6—C7—C7A—C3A	−0.6 (4)
C10—C9—C3—C3A	−76.4 (3)	C3A—C3—N2—O1	1.3 (3)
Cl—C9—C3—C3A	48.4 (3)	C9—C3—N2—O1	−175.9 (2)
N2—C3—C3A—C7A	−0.9 (3)	C3A—C7A—O1—N2	0.7 (3)
C9—C3—C3A—C7A	175.7 (2)	C7—C7A—O1—N2	−178.4 (2)
N2—C3—C3A—C4	177.7 (3)	C3—N2—O1—C7A	−1.2 (3)