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# Isopropyl 3-oxo-2,3-dihydro-1,2-benzothiazole-2-carboxylate

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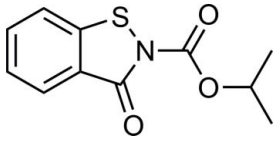
Key indicators: single-crystal X-ray study; $T$ = 153 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.039; $wR$ factor = 0.078; data-to-parameter ratio = 19.7.

The title compound, $C_{11}H_{11}NO_3S$, was synthesized by the reaction of benzo[*d*]isothiazol-3(2*H*)-one with isopropanol in toluene. The benzoisothiazolone ring system is essentially planar, with a mean deviation of 0.018 (2) Å from the least–squares plane defined by the nine constituent atoms. In the crystal, molecules are linked by weak intermolecular C—H···O hydrogen bonds.

## Related literature

For background to the sythesis of benzoisothiazolone derivatives, see: Davis (1972); Elgazwy & Abdel-Sattar (2003). For the biological activity of 1, 2–benzoisothiazolone derivatives, see: Taubert *et al.* (2002). For structural studies of related alkyl 3-oxo-2,3-dihydro-1,2-benzothiazole-2-carboxylate derivatives, see: Wang *et al.* (2011*a*,*b*).



## Experimental

### Crystal data

$C_{11}H_{11}NO_3S$
$M_r$ = 237.27
Orthorhombic, $P2_12_12_1$
$a$ = 4.6218 (19) Å
$b$ = 11.621 (5) Å
$c$ = 20.510 (9) Å
$V$ = 1101.6 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 153 K
0.68 × 0.12 × 0.07 mm

### Data collection

Rigaku AFC10/Saturn724+ diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.830, $T_{max}$ = 0.980
9436 measured reflections
2897 independent reflections
2245 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.078
$S$ = 1.00
2897 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$
Absolute structure: Flack, (1983), 1150 Friedel pairs
Flack parameter: −0.02 (8)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2···O1$^{i}$ | 0.95 | 2.47 | 3.225 (3) | 137 |

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

Data collection: *CrystalClear* (Rigaku, 2008); 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* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2199).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o2477 [ **doi:10.1107/S1600536811034209** ]

# Isopropyl 3-oxo-2,3-dihydro-1,2-benzothiazole-2-carboxylate

**X. Wang, Q. Lin and J. Yang**

## Comment

1,2-benzoisothiazol-3(2*H*)-ones are a class of compounds with a wide spectrum of biological activities (Davis, 1972; Elgazwy & Abdel-Sattar, 2003). 1, 2-Benzisothiazolone derivatives have been reported to possess high antibacterial and antifungal activity (Taubert *et al.*, 2002). As a part of our ongoing study of the substituent effect on the solid state structures of alkyl 3-oxo-2,3-dihydro-1,2-benzothiazole-2-carboxylate analogues (Wang, *et al.*, 2011*a*,*b*), we report herein the crystal structure of the title compound.

The title compound crystallizes as the non–centrosymmetric space group $P_{21\,21\,21}$ in spite of having no asymmetric C atoms. In the title molecule (Fig. 1), the benzoisothiazolone ring system is essentially planar, with a mean deviation of 0.018 (2) Å from the least–squares plane defined by the nine constituent atoms and the C8–C2–C9–C11 torsion angle is 156.63 (18)°. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds between a benzene H atom and the O atom of the carbonyl group (Table 1; C2—H2···O1$^{i}$).

## Experimental

A solution (20 ml) containing benzo[*d*]isothiazol-3(2*H*)-one (1.51 g, 0.01 mol) was added dropwise to a solution of isopropanol (0.61 g, 0.01 mol) and bis(triehloromethyl)Carbonate in toluene (20 ml) under stirring on an ice-water bath. The reaction mixture was stirred at room temperature for 4.5 h to afford the title compound (1.72 g, yield 72.6%). Single crystals suitable for X-ray measurements were obtained by recrystallization of the title compound from cyclohexane at room temperature.

## Refinement

The H atoms were placed at calculated positions and refined in riding mode, with the carrier atom–H distances = 0.95 Å for aryl, 0.99Å for methylene, 0.98 Å for the methyl. The *U*iso values were constrained to be 1.5*U*eq of the carrier atom for the methyl H atoms and 1.2*U*eq for the remaining H atoms.

## Figures

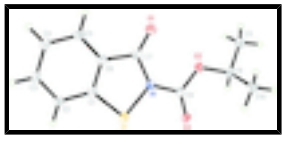

Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

### Isopropyl 3-oxo-2,3-dihydro-1,2-benzothiazole-2-carboxylate

*Crystal data*

| | |
|---|---|
| $C_{11}H_{11}NO_3S$ | $F(000) = 496$ |
| $M_r = 237.27$ | $D_x = 1.431$ Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 3268 reflections |
| $a = 4.6218$ (19) Å | $\theta = 2.7$–$29.1°$ |
| $b = 11.621$ (5) Å | $\mu = 0.28$ mm$^{-1}$ |
| $c = 20.510$ (9) Å | $T = 153$ K |
| $V = 1101.6$ (8) Å$^3$ | Prism, colorless |
| $Z = 4$ | 0.68 × 0.12 × 0.07 mm |

*Data collection*

| | |
|---|---|
| AFC10/Saturn724+ diffractometer | 2897 independent reflections |
| Radiation source: Rotating Anode | 2245 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.045$ |
| Detector resolution: 28.5714 pixels mm$^{-1}$ | $\theta_{max} = 29.1°$, $\theta_{min} = 3.5°$ |
| phi and ω scans | $h = -6 \rightarrow 6$ |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | $k = -14 \rightarrow 15$ |
| $T_{min} = 0.830$, $T_{max} = 0.980$ | $l = -28 \rightarrow 26$ |
| 9436 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | H-atom parameters constrained |
| $wR(F^2) = 0.078$ | $w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 0.116P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.00$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2897 reflections | $\Delta\rho_{max} = 0.26$ e Å$^{-3}$ |
| 147 parameters | $\Delta\rho_{min} = -0.22$ e Å$^{-3}$ |
| 0 restraints | Absolute structure: Flack, (1983), 1150 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: −0.02 (8) |

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.56113 (12) | 0.76406 (4) | 0.72970 (2) | 0.02649 (13) |
| O1 | 0.3920 (3) | 0.45795 (12) | 0.67074 (7) | 0.0339 (4) |
| O2 | 0.7876 (3) | 0.55858 (12) | 0.59264 (7) | 0.0289 (3) |
| O3 | 0.9282 (3) | 0.73722 (11) | 0.62359 (6) | 0.0303 (3) |
| N1 | 0.5743 (4) | 0.64449 (13) | 0.67914 (8) | 0.0231 (4) |
| C1 | 0.3073 (4) | 0.69457 (17) | 0.77902 (10) | 0.0258 (5) |
| C2 | 0.1822 (4) | 0.73839 (18) | 0.83559 (10) | 0.0285 (5) |
| H2 | 0.2327 | 0.8124 | 0.8516 | 0.034* |
| C3 | −0.0175 (5) | 0.67062 (18) | 0.86754 (11) | 0.0333 (6) |
| H3 | −0.1053 | 0.6986 | 0.9063 | 0.040* |
| C4 | −0.0940 (5) | 0.56146 (18) | 0.84420 (10) | 0.0319 (5) |
| H4 | −0.2360 | 0.5175 | 0.8666 | 0.038* |
| C5 | 0.0350 (5) | 0.51759 (17) | 0.78915 (10) | 0.0283 (5) |
| H5 | −0.0128 | 0.4428 | 0.7738 | 0.034* |
| C6 | 0.2375 (5) | 0.58518 (16) | 0.75632 (10) | 0.0236 (4) |
| C7 | 0.3987 (4) | 0.55027 (18) | 0.69814 (10) | 0.0246 (4) |
| C8 | 0.7810 (5) | 0.65258 (17) | 0.62952 (10) | 0.0248 (5) |
| C9 | 0.9960 (4) | 0.56000 (18) | 0.53842 (10) | 0.0293 (5) |
| H9 | 1.1790 | 0.5981 | 0.5529 | 0.035* |
| C10 | 0.8682 (6) | 0.62614 (19) | 0.48198 (11) | 0.0400 (6) |
| H10A | 0.6858 | 0.5902 | 0.4687 | 0.048* |
| H10B | 1.0041 | 0.6254 | 0.4453 | 0.048* |
| H10C | 0.8318 | 0.7058 | 0.4954 | 0.048* |
| C11 | 1.0554 (6) | 0.43512 (19) | 0.52321 (12) | 0.0432 (6) |
| H11A | 1.1449 | 0.3982 | 0.5611 | 0.052* |
| H11B | 1.1866 | 0.4299 | 0.4858 | 0.052* |
| H11C | 0.8731 | 0.3961 | 0.5128 | 0.052* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0236 (2) | 0.0281 (3) | 0.0277 (2) | −0.0018 (2) | 0.0024 (2) | −0.0002 (2) |
| O1 | 0.0339 (9) | 0.0294 (8) | 0.0386 (9) | −0.0041 (7) | 0.0053 (8) | −0.0039 (7) |
| O2 | 0.0272 (8) | 0.0338 (8) | 0.0256 (8) | −0.0021 (7) | 0.0072 (6) | −0.0037 (7) |
| O3 | 0.0312 (8) | 0.0314 (8) | 0.0284 (7) | −0.0096 (8) | 0.0033 (7) | −0.0001 (6) |
| N1 | 0.0192 (8) | 0.0240 (8) | 0.0261 (9) | −0.0014 (8) | 0.0021 (8) | −0.0011 (7) |
| C1 | 0.0184 (10) | 0.0304 (11) | 0.0286 (11) | 0.0032 (8) | −0.0010 (9) | 0.0056 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0284 (11) | 0.0292 (11) | 0.0277 (10) | −0.0002 (10) | 0.0001 (9) | −0.0004 (9) |
| C3 | 0.0330 (14) | 0.0401 (13) | 0.0267 (11) | 0.0055 (10) | 0.0060 (9) | 0.0043 (9) |
| C4 | 0.0271 (12) | 0.0346 (12) | 0.0341 (12) | 0.0014 (11) | 0.0050 (10) | 0.0105 (10) |
| C5 | 0.0234 (11) | 0.0239 (11) | 0.0376 (12) | 0.0004 (9) | −0.0024 (10) | 0.0040 (9) |
| C6 | 0.0181 (10) | 0.0255 (11) | 0.0273 (11) | 0.0031 (8) | −0.0042 (8) | 0.0048 (8) |
| C7 | 0.0172 (10) | 0.0290 (11) | 0.0275 (10) | −0.0003 (9) | −0.0023 (9) | 0.0047 (8) |
| C8 | 0.0218 (11) | 0.0313 (12) | 0.0215 (10) | 0.0023 (9) | −0.0029 (9) | 0.0028 (9) |
| C9 | 0.0262 (13) | 0.0373 (12) | 0.0244 (10) | −0.0021 (10) | 0.0055 (9) | −0.0009 (9) |
| C10 | 0.0405 (16) | 0.0507 (14) | 0.0289 (12) | −0.0036 (12) | −0.0017 (11) | 0.0002 (11) |
| C11 | 0.0464 (15) | 0.0454 (13) | 0.0377 (13) | 0.0011 (14) | 0.0115 (13) | −0.0039 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—N1 | 1.7349 (17) | C4—C5 | 1.375 (3) |
| S1—C1 | 1.747 (2) | C4—H4 | 0.9500 |
| O1—C7 | 1.212 (2) | C5—C6 | 1.395 (3) |
| O2—C8 | 1.329 (2) | C5—H5 | 0.9500 |
| O2—C9 | 1.472 (2) | C6—C7 | 1.464 (3) |
| O3—C8 | 1.202 (2) | C9—C11 | 1.509 (3) |
| N1—C8 | 1.399 (3) | C9—C10 | 1.510 (3) |
| N1—C7 | 1.418 (3) | C9—H9 | 1.0000 |
| C1—C6 | 1.392 (3) | C10—H10A | 0.9800 |
| C1—C2 | 1.393 (3) | C10—H10B | 0.9800 |
| C2—C3 | 1.379 (3) | C10—H10C | 0.9800 |
| C2—H2 | 0.9500 | C11—H11A | 0.9800 |
| C3—C4 | 1.401 (3) | C11—H11B | 0.9800 |
| C3—H3 | 0.9500 | C11—H11C | 0.9800 |
| N1—S1—C1 | 89.97 (9) | O1—C7—C6 | 127.63 (19) |
| C8—O2—C9 | 115.85 (16) | N1—C7—C6 | 107.53 (17) |
| C8—N1—C7 | 130.00 (17) | O3—C8—O2 | 127.0 (2) |
| C8—N1—S1 | 113.89 (13) | O3—C8—N1 | 121.00 (19) |
| C7—N1—S1 | 115.74 (14) | O2—C8—N1 | 112.00 (17) |
| C6—C1—C2 | 121.1 (2) | O2—C9—C11 | 105.33 (17) |
| C6—C1—S1 | 112.58 (15) | O2—C9—C10 | 109.20 (17) |
| C2—C1—S1 | 126.31 (17) | C11—C9—C10 | 113.71 (19) |
| C3—C2—C1 | 117.7 (2) | O2—C9—H9 | 109.5 |
| C3—C2—H2 | 121.1 | C11—C9—H9 | 109.5 |
| C1—C2—H2 | 121.1 | C10—C9—H9 | 109.5 |
| C2—C3—C4 | 121.6 (2) | C9—C10—H10A | 109.5 |
| C2—C3—H3 | 119.2 | C9—C10—H10B | 109.5 |
| C4—C3—H3 | 119.2 | H10A—C10—H10B | 109.5 |
| C5—C4—C3 | 120.5 (2) | C9—C10—H10C | 109.5 |
| C5—C4—H4 | 119.8 | H10A—C10—H10C | 109.5 |
| C3—C4—H4 | 119.8 | H10B—C10—H10C | 109.5 |
| C4—C5—C6 | 118.6 (2) | C9—C11—H11A | 109.5 |
| C4—C5—H5 | 120.7 | C9—C11—H11B | 109.5 |
| C6—C5—H5 | 120.7 | H11A—C11—H11B | 109.5 |
| C1—C6—C5 | 120.5 (2) | C9—C11—H11C | 109.5 |
| C1—C6—C7 | 114.09 (18) | H11A—C11—H11C | 109.5 |

| | | | |
|---|---|---|---|
| C5—C6—C7 | 125.36 (18) | H11B—C11—H11C | 109.5 |
| O1—C7—N1 | 124.83 (19) | | |
| C1—S1—N1—C8 | −175.20 (15) | S1—N1—C7—O1 | −175.99 (17) |
| C1—S1—N1—C7 | −1.47 (16) | C8—N1—C7—C6 | 175.40 (19) |
| N1—S1—C1—C6 | −0.54 (15) | S1—N1—C7—C6 | 2.9 (2) |
| N1—S1—C1—C2 | 178.93 (19) | C1—C6—C7—O1 | 175.6 (2) |
| C6—C1—C2—C3 | −1.3 (3) | C5—C6—C7—O1 | −2.9 (3) |
| S1—C1—C2—C3 | 179.25 (17) | C1—C6—C7—N1 | −3.3 (2) |
| C1—C2—C3—C4 | −0.2 (3) | C5—C6—C7—N1 | 178.28 (19) |
| C2—C3—C4—C5 | 1.6 (3) | C9—O2—C8—O3 | −0.8 (3) |
| C3—C4—C5—C6 | −1.6 (3) | C9—O2—C8—N1 | 179.12 (16) |
| C2—C1—C6—C5 | 1.4 (3) | C7—N1—C8—O3 | −173.8 (2) |
| S1—C1—C6—C5 | −179.12 (16) | S1—N1—C8—O3 | −1.2 (3) |
| C2—C1—C6—C7 | −177.15 (18) | C7—N1—C8—O2 | 6.3 (3) |
| S1—C1—C6—C7 | 2.3 (2) | S1—N1—C8—O2 | 178.90 (13) |
| C4—C5—C6—C1 | 0.1 (3) | C8—O2—C9—C11 | 156.63 (18) |
| C4—C5—C6—C7 | 178.46 (19) | C8—O2—C9—C10 | −80.9 (2) |
| C8—N1—C7—O1 | −3.5 (3) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···O1$^{i}$ | 0.95 | 2.47 | 3.225 (3) | 137. |

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

**Fig. 1**