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2-(Hydroxymethyl)-1,2-benzothiazol-3(2*H*)-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.058
wR factor = 0.105
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_8H_7NO_2S$, the benzisothiazolone ring system is planar, with a maximum deviation from the mean plane of 0.038 (2) Å for the N atom. Weak intermolecular hydrogen bonds and a π–π stacking interaction stabilize the crystal structure.

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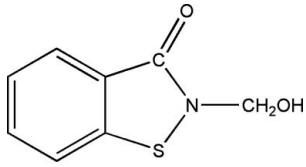
Comment

It has been reported that isothiazolones and heterocyclic bioisosteric derivatives are potent industrial microbiocides with antifungal and antibacterial activities (Taubert *et al.*, 2002). These compounds are also highly potent platelet aggregation inhibitors (Vicini *et al.*, 2000), and show anti-inflammatory, analgesic and antipyretic activities (Bordi *et al.*, 1992). In view of this, we report here the crystal structure of the title compound, (I) (Fig. 1).



(I)

Bond lengths and angles of the benzisothiazolone ring system (Table 1) are in good agreement with the values quoted in a previous report (Kim *et al.*, 1996). The benzisothiazolone ring system is planar, with a maximum deviation from the mean plane of 0.038 (2) Å for atom N1.

The crystal structure of (I) is stabilized by weak intermolecular hydrogen bonds (Table 2) and π–π stacking interactions. The isothiazolone rings of centrosymmetrically

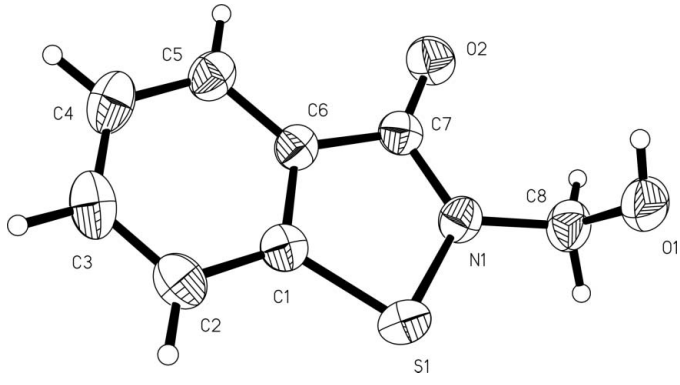


Figure 1
View of the title compound, with displacement ellipsoids drawn at the 40% probability level.

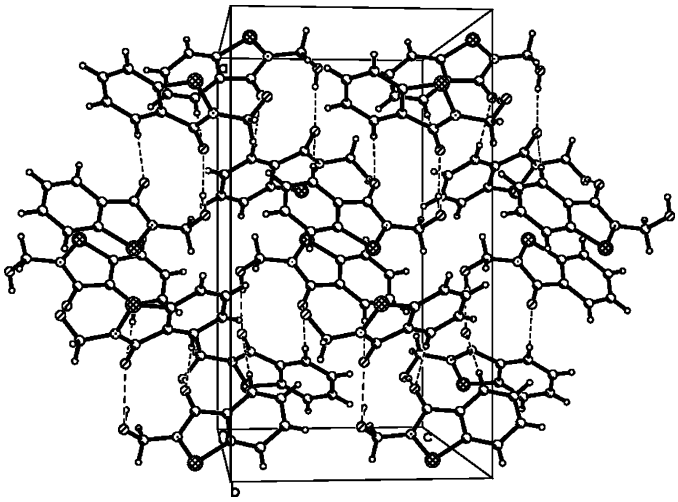


Figure 2
A packing diagram of the molecule of the title compound, viewed approximately down the *b* axis. Hydrogen bonds are shown as dashed lines.

related molecules at (*x*, *y*, *z*) and (−*x*, −*y*, −*z*) stack with a distance of 3.496 (3) Å between the ring centroids.

Experimental

A mixture of benzisothiazolone (0.02 mol) and polyoxymethylene (0.022 mol) was stirred in refluxing chloroform (10 ml) for 5 h at 334 K to afford the title compound (3.13 g, yield 87%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_8H_7NO_2S$
M_r = 181.21
Tetragonal, $I4_1/a$
a = 17.856 (7) Å
c = 9.955 (2) Å
V = 3174.0 (19) Å^3
Z = 16
D_x = 1.517 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 4–14°
μ = 0.36 mm^{-1}
T = 293 (2) K
Block, colourless
0.25 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.915, T_{max} = 0.942
6764 measured reflections
1704 independent reflections
1365 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 27.0°
$h = -22 \rightarrow 22$
$k = -22 \rightarrow 22$
$l = 0 \rightarrow 11$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.105
S = 1.12
1704 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.6111P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0021 (5)

Table 1
Selected geometric parameters (Å, °).

S1—N1	1.7119 (17)	N1—C7	1.372 (2)
S1—C1	1.7335 (18)	N1—C8	1.456 (2)
O1—C8	1.391 (2)	C7—O2	1.234 (2)
O2—C7	1.234 (2)		
N1—S1—C1	90.51 (8)	C8—N1—S1	119.23 (13)
C7—N1—C8	123.83 (16)	O1—C8—N1	112.77 (15)
C7—N1—S1	116.09 (11)		
C1—S1—N1—C7	2.77 (13)	N1—S1—C1—C2	179.03 (16)
C1—S1—N1—C8	172.64 (14)	C7—N1—C8—O1	94.6 (2)
N1—S1—C1—C6	−2.26 (13)	S1—N1—C8—O1	−74.5 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2^{i}	0.82	1.97	2.774 (2)	169
C5—H5A···O2^{ii}	0.93	2.57	3.492 (3)	171

Symmetry codes: (i) $y+\frac{1}{4}, -x+\frac{1}{4}, z+\frac{1}{4}$; (ii) $-y+\frac{1}{4}, x-\frac{1}{4}, z-\frac{1}{4}$.

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å and O—H = 0.82 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) for the aryl and methylene H atoms and 1.5U_{eq}(O) for the hydroxy H atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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