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3-(1,3-Benzoxazol-2-ylsulfanyl)-4*H*-chromen-4-one

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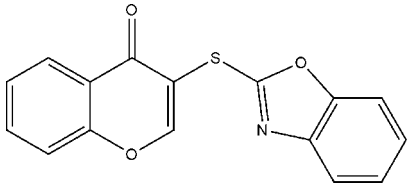
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.060; wR factor = 0.159; data-to-parameter ratio = 15.5.

In the molecule of the title compound, $C_{16}H_9NO_3S$, the two fused ring systems are each planar and make a dihedral angle of 78.0 (1)° with each other. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules into chains along the b axis and there are also π–π stacking interactions. The distance between the adjacent ring centroids of the benzoxazole system is 3.89 (1) Å (symmetry code linking the adjacent rings: $1-x$, $1-y$, $1-z$). A further interaction occurs between two adjacent six-membered benzoxazole benzene rings (symmetry code: $1-x$, $-y$, $1-z$), with a centroid -to-centroid distance of 3.93 (1) Å.

Related literature

For general background, see: Ren *et al.* (2003); Kim *et al.* (2004); Allen *et al.* (1987); Janiak (2000). For related literature, see: Huang *et al.* (2005).



Experimental

Crystal data

$C_{16}H_9NO_3S$
M_r = 295.30
Monoclinic, $P2_1/c$
a = 13.3357 (10) Å
b = 6.7749 (5) Å
c = 15.0185 (11) Å
β = 107.417 (1)°
V = 1294.68 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 291 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4 K CCD area-detector diffractometer
Absorption correction: none
9560 measured reflections
2939 independent reflections
2128 reflections with $I > 2\sigma(I)$
R_{int} = 0.118

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.159
S = 0.99
2939 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O2^{i}	0.93	2.51	3.231 (3)	135

Symmetry code: (i) $x, y-1, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2248).

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supplementary materials

Acta Cryst. (2007). E**63**, o2984 [**doi:10.1107/S1600536807023914**]

3-(1,3-Benzoxazol-2-ylsulfanyl)-4*H*-chromen-4-one

W. Huang

Comment

Flavonoids, occurring widely throughout the plant kingdom, are one of the most representative families of plant secondary metabolites and display a remarkable spectrum of biological activities. They are one of the most important groups of biological compounds in nature, and are used as a synthetic lead for drug discovery (Ren *et al.*, 2003; Kim *et al.*, 2004). The title compound, (I), is a flavonoid derivative with bioactive heterocyclic thioether subunit. We herein report its crystal structure.

In the molecule of the title compound, (I), (Fig. 1), the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987).

The rings A (C1—C6), B (O1/C1/C6—C9), C (N1/O3/C10/C11/C16) and D (C11—C16) are, of course, planar and the dihedral angles between them are A/B = 1.0 (1)° and C/D = 1.0 (1)°. So, the rings A, B and C, D are coplanar and they are also oriented at a dihedral angle of 78.0 (1)°.

In the crystal structure, the intermolecular C—H···O hydrogen bonds link the molecules into chains along the *b* axis (Fig. 2), in which they may be effective in the stabilization of the structure. Further stability is provided by the offset π-π stacking interactions (Janiak, 2000) involving the adjacent coplanar rings C and D with centroid···centroid (symmetry code: 1 − *x*, 1 − *y*, 1 − *z*) distance of 3.89 (1) Å, beside of the adjacent D rings with centroid···centroid (symmetry code: 1 − *x*, −*y*, 1 − *z*) distance of 3.93 (1) Å.

Experimental

The title compound, (I), was synthesized according to the literature method (Huang *et al.*, 2005). Crystals suitable for X-ray analysis were grown from dichloromethane at 277 K.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

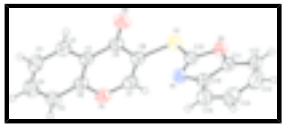

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

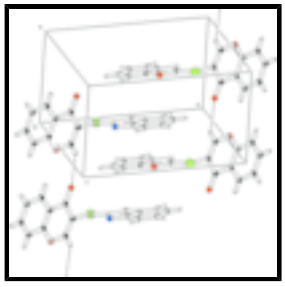

Fig. 2. A packing diagram for (I). H bonds are shown as dashed lines.

3-(1,3-Benzoxazol-2-ylsulfanyl)-4*H*-chromen-4-one

Crystal data

$C_{16}H_9NO_3S$	F_{000} = 608
M_r = 295.30	D_x = 1.515 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2673 reflections
a = 13.3357 (10) Å	θ = 2.8–25.4º
b = 6.7749 (5) Å	μ = 0.26 mm^{-1}
c = 15.0185 (11) Å	T = 291 (2) K
β = 107.417 (1)º	Plate, yellow
V = 1294.68 (17) Å^3	0.20 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2128 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.118
Monochromator: graphite	θ_{max} = 27.5º
T = 291(2) K	θ_{min} = 1.6º
φ and ω scans	h = −17→14
Absorption correction: none	k = −8→8
9560 measured reflections	l = −19→17
2939 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.060	H-atom parameters constrained
$wR(F^2)$ = 0.159	$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = <0.001
2939 reflections	$\Delta\rho_{max}$ = 0.45 e Å^{-3}

190 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.25607 (5)	0.15017 (9)	0.31455 (4)	0.0564 (2)
O1	0.00612 (12)	−0.0770 (2)	0.36603 (10)	0.0529 (4)
O2	0.11610 (13)	0.4808 (2)	0.35113 (11)	0.0617 (5)
O3	0.44360 (12)	0.2234 (2)	0.42736 (11)	0.0546 (4)
N1	0.32159 (15)	0.2063 (3)	0.50334 (13)	0.0501 (5)
C1	−0.01555 (17)	0.2751 (3)	0.37804 (13)	0.0429 (5)
C2	−0.07754 (18)	0.4293 (4)	0.39490 (15)	0.0529 (6)
H2	−0.0564	0.5596	0.3928	0.064*
C3	−0.1697 (2)	0.3877 (4)	0.41463 (17)	0.0632 (7)
H3	−0.2107	0.4899	0.4263	0.076*
C4	−0.2016 (2)	0.1924 (4)	0.41714 (17)	0.0645 (7)
H4	−0.2641	0.1663	0.4304	0.077*
C5	−0.14377 (18)	0.0390 (4)	0.40063 (16)	0.0558 (6)
H5	−0.1657	−0.0909	0.4025	0.067*
C6	−0.05054 (18)	0.0830 (3)	0.38089 (14)	0.0463 (5)
C7	0.09752 (18)	−0.0436 (3)	0.34882 (14)	0.0490 (5)
H7	0.1357	−0.1527	0.3399	0.059*
C8	0.13791 (17)	0.1350 (3)	0.34352 (15)	0.0447 (5)
C9	0.08359 (18)	0.3143 (3)	0.35709 (14)	0.0444 (5)
C10	0.34169 (17)	0.1960 (3)	0.42519 (16)	0.0487 (6)
C11	0.49506 (18)	0.2573 (3)	0.52130 (17)	0.0509 (6)
C12	0.5994 (2)	0.3002 (4)	0.5648 (2)	0.0646 (7)
H12	0.6483	0.3096	0.5319	0.078*
C13	0.6269 (2)	0.3284 (4)	0.6604 (2)	0.0710 (8)
H13	0.6963	0.3577	0.6929	0.085*
C14	0.5543 (2)	0.3142 (4)	0.7084 (2)	0.0735 (8)
H14	0.5762	0.3313	0.7728	0.088*
C15	0.4496 (2)	0.2751 (4)	0.66347 (19)	0.0678 (7)
H15	0.4005	0.2684	0.6962	0.081*
C16	0.42064 (18)	0.2463 (3)	0.56834 (16)	0.0496 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0623 (4)	0.0622 (4)	0.0489 (4)	0.0040 (3)	0.0232 (3)	−0.0020 (3)
O1	0.0595 (10)	0.0400 (8)	0.0574 (10)	−0.0033 (7)	0.0149 (8)	−0.0003 (7)
O2	0.0705 (12)	0.0417 (9)	0.0777 (12)	−0.0042 (8)	0.0298 (9)	−0.0009 (8)
O3	0.0522 (10)	0.0552 (9)	0.0646 (11)	0.0072 (7)	0.0298 (8)	0.0047 (8)
N1	0.0469 (11)	0.0583 (11)	0.0484 (11)	−0.0007 (9)	0.0194 (9)	0.0017 (9)
C1	0.0502 (13)	0.0444 (11)	0.0315 (11)	0.0013 (9)	0.0081 (9)	−0.0007 (8)
C2	0.0617 (15)	0.0492 (12)	0.0482 (13)	0.0050 (11)	0.0170 (11)	0.0012 (10)
C3	0.0627 (17)	0.0728 (17)	0.0538 (15)	0.0159 (14)	0.0169 (12)	−0.0026 (12)
C4	0.0550 (15)	0.088 (2)	0.0516 (15)	−0.0049 (14)	0.0172 (12)	−0.0011 (13)
C5	0.0549 (15)	0.0601 (15)	0.0506 (13)	−0.0097 (11)	0.0130 (11)	0.0018 (11)
C6	0.0542 (13)	0.0460 (11)	0.0330 (11)	−0.0025 (10)	0.0044 (9)	−0.0001 (9)
C7	0.0578 (14)	0.0416 (12)	0.0444 (12)	0.0044 (10)	0.0105 (10)	−0.0010 (9)
C8	0.0512 (13)	0.0432 (11)	0.0375 (11)	0.0009 (9)	0.0099 (9)	−0.0014 (8)
C9	0.0549 (13)	0.0406 (11)	0.0349 (11)	−0.0007 (9)	0.0094 (9)	0.0022 (8)
C10	0.0489 (14)	0.0415 (11)	0.0592 (15)	0.0062 (9)	0.0215 (11)	0.0046 (10)
C11	0.0477 (13)	0.0412 (11)	0.0655 (16)	0.0082 (9)	0.0197 (11)	0.0070 (10)
C12	0.0466 (14)	0.0549 (14)	0.098 (2)	0.0088 (11)	0.0299 (14)	0.0077 (14)
C13	0.0525 (16)	0.0570 (15)	0.092 (2)	0.0069 (12)	0.0039 (15)	−0.0015 (14)
C14	0.0648 (18)	0.0763 (19)	0.0681 (19)	0.0070 (14)	0.0030 (15)	−0.0031 (14)
C15	0.0619 (17)	0.0843 (19)	0.0571 (16)	0.0021 (14)	0.0176 (13)	0.0028 (13)
C16	0.0475 (13)	0.0504 (13)	0.0542 (14)	0.0050 (10)	0.0203 (11)	0.0048 (10)

Geometric parameters (Å, °)

S1—C10	1.739 (2)	C4—C5	1.361 (4)
S1—C8	1.759 (2)	C6—C5	1.394 (3)
O1—C6	1.378 (3)	C7—H7	0.9300
O1—C7	1.339 (3)	C8—C7	1.337 (3)
O3—C10	1.362 (3)	C8—C9	1.460 (3)
O3—C11	1.391 (3)	C9—O2	1.221 (2)
N1—C10	1.282 (3)	C11—C12	1.380 (4)
N1—C16	1.414 (3)	C11—C12	1.380 (4)
C1—C2	1.401 (3)	C12—H12	0.9300
C1—C6	1.387 (3)	C13—C12	1.384 (4)
C1—C9	1.472 (3)	C13—H13	0.9300
C2—C3	1.377 (3)	C13—C14	1.373 (4)
C2—H2	0.9300	C14—H14	0.9300
C5—H5	0.9300	C14—C15	1.383 (4)
C3—H3	0.9300	C15—H15	0.9300
C4—C3	1.394 (4)	C16—C11	1.382 (3)
C4—H4	0.9300	C16—C15	1.378 (3)
C10—S1—C8	98.90 (10)	C7—C8—S1	118.32 (17)
C7—O1—C6	118.26 (16)	C9—C8—S1	120.31 (16)
C10—O3—C11	103.44 (16)	O2—C9—C8	123.8 (2)

C10—N1—C16	103.55 (18)	O2—C9—C1	122.9 (2)
C6—C1—C2	118.1 (2)	C8—C9—C1	113.23 (18)
C6—C1—C9	120.54 (19)	N1—C10—O3	116.8 (2)
C2—C1—C9	121.3 (2)	N1—C10—S1	128.83 (18)
C3—C2—C1	120.0 (2)	O3—C10—S1	114.33 (16)
C3—C2—H2	120.0	C12—C11—C16	123.1 (2)
C1—C2—H2	120.0	C12—C11—O3	129.5 (2)
C2—C3—C4	120.0 (2)	C16—C11—O3	107.3 (2)
C2—C3—H3	120.0	C11—C12—C13	115.9 (2)
C4—C3—H3	120.0	C11—C12—H12	122.1
C5—C4—C3	121.7 (2)	C13—C12—H12	122.1
C5—C4—H4	119.1	C14—C13—C12	121.7 (3)
C3—C4—H4	119.1	C14—C13—H13	119.1
C4—C5—C6	117.8 (2)	C12—C13—H13	119.1
C4—C5—H5	121.1	C13—C14—C15	121.7 (3)
C6—C5—H5	121.1	C13—C14—H14	119.2
O1—C6—C1	121.8 (2)	C15—C14—H14	119.2
O1—C6—C5	115.7 (2)	C16—C15—C14	117.5 (3)
C1—C6—C5	122.5 (2)	C16—C15—H15	121.3
C8—C7—O1	124.8 (2)	C14—C15—H15	121.3
C8—C7—H7	117.6	C15—C16—C11	120.1 (2)
O1—C7—H7	117.6	C15—C16—N1	131.0 (2)
C7—C8—C9	121.3 (2)	C11—C16—N1	108.8 (2)
C10—S1—C8—C7	−102.78 (19)	C2—C1—C9—C8	178.82 (18)
C10—S1—C8—C9	79.95 (19)	C1—C2—C3—C4	−0.5 (4)
C8—S1—C10—N1	2.5 (2)	C5—C4—C3—C2	0.1 (4)
C8—S1—C10—O3	−177.82 (15)	C3—C4—C5—C6	0.0 (4)
C7—O1—C6—C1	0.3 (3)	O1—C6—C5—C4	179.1 (2)
C7—O1—C6—C5	−178.55 (18)	C1—C6—C5—C4	0.3 (3)
C6—O1—C7—C8	−1.0 (3)	C9—C8—C7—O1	0.3 (4)
C11—O3—C10—N1	−0.5 (2)	S1—C8—C7—O1	−176.91 (16)
C11—O3—C10—S1	179.82 (14)	C7—C8—C9—O2	−178.5 (2)
C10—O3—C11—C12	−177.9 (2)	S1—C8—C9—O2	−1.3 (3)
C10—O3—C11—C16	0.5 (2)	C7—C8—C9—C1	1.0 (3)
C16—N1—C10—O3	0.3 (3)	S1—C8—C9—C1	178.19 (14)
C16—N1—C10—S1	179.92 (17)	C16—C11—C12—C13	1.3 (3)
C10—N1—C16—C15	179.4 (3)	O3—C11—C12—C13	179.4 (2)
C10—N1—C16—C11	0.1 (2)	C14—C13—C12—C11	0.0 (4)
C6—C1—C2—C3	0.7 (3)	C12—C13—C14—C15	−1.4 (4)
C9—C1—C2—C3	−179.8 (2)	C13—C14—C15—C16	1.4 (4)
C2—C1—C6—O1	−179.36 (18)	C15—C16—C11—C12	−1.3 (4)
C9—C1—C6—O1	1.1 (3)	N1—C16—C11—C12	178.1 (2)
C2—C1—C6—C5	−0.6 (3)	C15—C16—C11—O3	−179.7 (2)
C9—C1—C6—C5	179.86 (19)	N1—C16—C11—O3	−0.3 (2)
C6—C1—C9—O2	177.8 (2)	C11—C16—C15—C14	−0.1 (4)
C2—C1—C9—O2	−1.7 (3)	N1—C16—C15—C14	−179.4 (2)
C6—C1—C9—C8	−1.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O2^{i}	0.93	2.51	3.231 (3)	135

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1

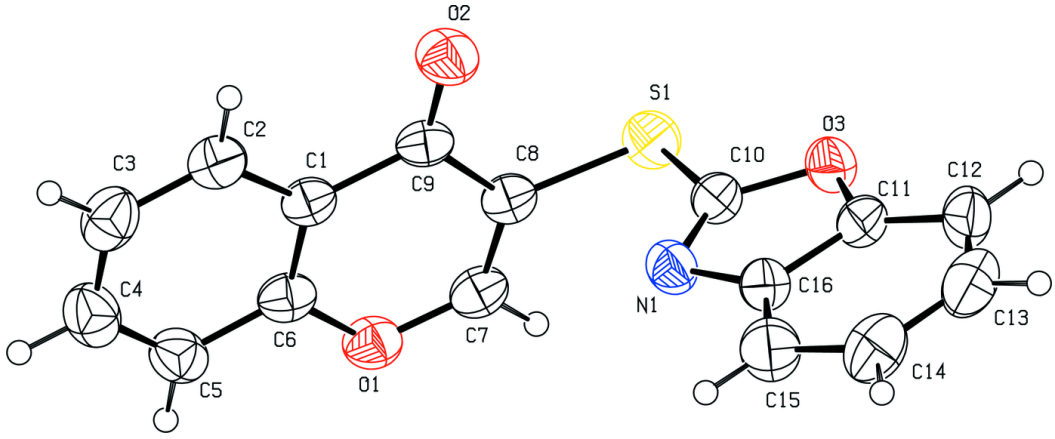

Fig. 2