

(7-chloro-2-oxo-2H-chromen-4-yl)methyldimethylcarbamodithioate

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ABSTRACT

In the title compound, $C_{13}H_{12}ClN O_2S_2$, the 2H-chromene ring system is planar, with a maximum deviation of 0.005 (2) Å. A short $H\cdots H$ contact of 2.3873 (1) Å is present and generate R^2 loops. In the crystal, molecules are link the stack along (100) plane by $C-H\cdots O$ hydrogen bonds. The crystal structure further stabilized by intermolecular $C-H\cdots S$ hydrogen bonds, $C-H\cdots \pi$ and $\pi-\pi$ interactions between fused benzene rings of chromene [shortest centroid-centroid distance = 3.6556 (12) Å].

Comment

Synthetic coumarins are widely used as aroma chemicals because of their odour strength, tenacity, stability to alkali and relatively cheap price; applications include use as a sweetener and fixative (in perfume); fragrance enhancers (for natural essential oils); blenders (in soaps and detergents); aroma enhancers (in tobacco); and for imparting pleasant odours to industrial products. The coumarins have been the subject of extensive studies because of their interesting biological activities and have, in fact, been used as therapeutic agents for the treatment of various diseases. Coumarins show quite diverse biological activities, including anticoagulant, anti-allergic, anthelmintic, diuretic, insecticidal and antibiotic properties (Trkovnik *et al.*, 1983); Rao *et al.*, 1981). The great electrophilicity of nitrogen atom compared to that of sulfur atom makes the latter more acidic and an active centre in the nucleophilic attack. The fact that, the sulfur anion formed is more stabilized by negative charge distribution. Furthermore, functionalized carbamates are an important class of compounds and their medicinal and biological properties warrant study (Dhooghe *et al.*, 2006). Organic dithiocarbamates are valuable synthetic intermediates (Boas *et al.*, 2004), which are ubiquitously found in a variety of biologically active compounds. Functionalization of the carbamate moiety offers an attractive method for the generation of derivatives, which may constitute interesting medicinal and biological properties (Fernandez *et al.*, 1995).

The asymmetric unit of (7-chloro-2-oxo-2H-chromen-4-yl)methyl dimethylcarbamodithioate is shown in Fig. 1. The 2H-chromene ring system is planar, with a maximum deviation of 0.005 (2) Å for the atom C13. A short $H14\cdots H18$ contact of 2.3873 (1) Å is present and generate R^2 loops. In the crystal, molecules are link the stack along (100) plane by C

$-H\cdots O$ hydrogen bonds. The crystal structure packing further stabilized by intermolecular $C16-H16A\cdots S3$ hydrogen bonds and $C_g(2)(C7-C12)\pi-\pi C_g(2)$ interactions between fused benzene rings of chromene [shortest centroid-centroid distance = 3.6556 (12) Å]. The packing of the molecules of the title compound (Fig. 2).

Synthesis and crystallization

All the chemicals used were of analytical reagent grade and were used directly without further purification. The title compound was synthesized according to the reported method (Mahabaleshwaraiah *et al.*, 2012). The compound is recrystallized by ethanol-chloroform mixture. Colourless needles of the title compound were grown from a mixed solution of Ethanol/Chloroform (V/V = 2/1) by slow evaporation at room temperature. Yield = 72%; m.p.: 405–407 K.

Refinement

All H atoms were positioned geometrically, with $C-H = 0.93$ Å for aromatic H, $C-H = 0.97$ Å for methylene

H and C

—H = 0.96 Å for methyl H, and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H and $U_{\text{iso}}(\text{H}) =$

1.2 $U_{\text{eq}}(\text{C})$ for all other H.

Table 1 Experimental details

Parameter	Data
Chemical formula	C ₁₃ H ₁₂ ClNO ₂ S ₂
<i>Mr</i>	313.81
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.7244 (4), 7.1157 (3), 20.0896 (9)
β (°)	94.404 (3)
<i>V</i> (Å ³)	1386.01 (10)
<i>Z</i>	4
Radiation type	Mo K α
μ (mm ⁻¹)	0.57
Crystal size (mm)	0.24 × 0.20 × 0.12
Data collection	—
Diffractometer	Bruker <i>SMART</i> CCD area-detector diffractometer
Absorption correction	ψ scan, <i>SADABS</i> (Sheldrick, 2007)
<i>T</i> _{min} , <i>T</i> _{max}	0.770, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	16144, 4752, 2810
<i>R</i> _{int}	0.029
(sin θ/λ) _{max} (Å ⁻¹)	0.749
Refinement	—
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.053, 0.148, 1.03
No. of reflections	4752
No. of parameters	172
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.33, -0.34

Computer programs: *SMART* (Bruker, 2001), *SAINT* (Bruker, 2001), *SAINT*, *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *ORTEP-3*

(Farrugia, 1997), *SHELXL97*.

Table 2 Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C16—H16A $\cdots$ S3 ⁱ	0.97	2.83	3.707 (2)	150
Symmetry code: (i) $-x, y+1/2, -z+1/2$.				

ACKNOWLEDGEMENTS

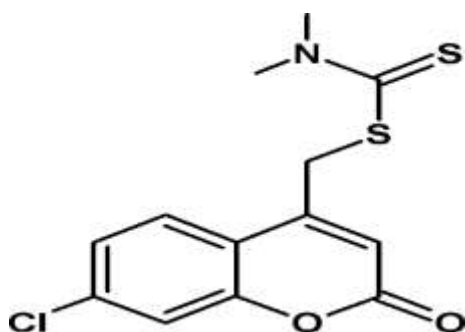
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Figure 1 Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.



supplementary materials

(7-chloro-2-oxo-2H-chromen-4-yl)methyldimethylcarbamodithioate

Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Crystal data

$C_{13}H_{12}ClNO_2S_2$

$M_r = 313.81$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1bc$

$a = 9.7244\ (4)\ \text{\AA}$



$$b = 7.1157 (3) \text{ \AA}$$

$$c = 20.0896 (9) \text{ \AA}$$

$$\beta = 94.404 (3)^\circ$$

$$V = 1386.01 (10) \text{ \AA}^3$$

$$Z = 4$$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube Graphite monochromator

ω and φ scans

Absorption correction: ψ scan

SADABS (Sheldrick, 2007)

$$T_{\min} = 0.770, T_{\max} = 1.000$$

Refinement

Refinement on F^2

Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.053$ $wR(F^2) = 0.148$

$$S = 1.03$$

4752 reflections

172 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Special details

Refinement $F(000) = 648$

$$D_x = 1.504 \text{ Mg m}^{-3}$$

Melting point: 407 K

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4752 reflections

$$\theta = 2.0\text{--}32.2^\circ \mu = 0.57 \text{ mm}^{-1} T = 296 \text{ K}$$

Plate, colourless

$$0.24 \times 0.20 \times 0.12 \text{ mm}$$



16144 measured reflections

4752 independent reflections 2810 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\text{max}} = 32.2^\circ$, $\theta_{\text{min}} = 2.0^\circ$

$h = -14 \rightarrow 14$

$k = -10 \rightarrow 10$

$l = -27 \rightarrow 30$

Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouringsites

H-atom parameters constrained

$w = 1/[\sigma^2(F^2) + (0.0631P)^2 + 0.4524P]$

where $P = (F^2 + 2F^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.33 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.34 \text{ e } \text{\AA}^{-3}$

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 $F^2 > 2\sigma(F^2)$ 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 ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	-0.17684 (7)	0.68938 (10)	0.60870 (3)	0.0644 (2)
S2	0.19843 (6)	0.93879 (9)	0.24696 (3)	0.05246 (18)
S3	0.25792 (7)	0.52240 (10)	0.23740 (3)	0.05584 (19)
O4	0.27368 (15)	0.7395 (2)	0.50557 (7)	0.0490 (4)
O5	0.48212 (17)	0.7569 (3)	0.47040 (9)	0.0675 (5)
N6	0.37618 (19)	0.7923 (3)	0.17127 (9)	0.0519 (5)
C7	-0.0833 (2)	0.7267 (3)	0.53956 (11)	0.0420 (5)
C8	-0.1506 (2)	0.7600 (3)	0.47814 (12)	0.0442 (5)
H8	-0.2464	0.7643	0.4731	0.053*
C9	-0.0740 (2)	0.7868 (3)	0.42394 (11)	0.0413 (5)
H9	-0.1193	0.8092	0.3822	0.050*
C10	0.0704 (2)	0.7809 (3)	0.43022 (10)	0.0349 (4)
C11	0.1331 (2)	0.7473 (3)	0.49381 (10)	0.0369 (4)
C12	0.0578 (2)	0.7199 (3)	0.54876 (11)	0.0442 (5)
H12	0.1017	0.6975	0.5908	0.053*



C13	0.15921 (19)	0.8082 (3)	0.37604 (10)	0.0369 (4)
C14	0.2965 (2)	0.8017 (3)	0.38969 (11)	0.0420 (5)
H14	0.3529	0.8212	0.355	0.050*
C15	0.3604 (2)	0.7660 (3)	0.45540 (11)	0.0456 (5)
C16	0.0936 (2)	0.8373 (4)	0.30681 (11)	0.0501 (6)
H16A	0.0133	0.9169	0.3098	0.060*
H16B	0.0609	0.7164	0.2898	0.060*
C17	0.2866 (2)	0.7428 (3)	0.21486 (10)	0.0416 (5)
C18	0.4621 (3)	0.6495 (5)	0.14198 (14)	0.0775 (9)
H18A	0.5207	0.7087	0.1118	0.116*
H18B	0.4041	0.5591	0.1181	0.116*
H18C	0.5179	0.5874	0.1769	0.116*
C19	0.4015 (3)	0.9850 (5)	0.15158 (15)	0.0725 (9)
H19A	0.4704	0.9867	0.1198	0.109*
H19B	0.4331	1.0569	0.1902	0.109*
H19C	0.3176	1.0388	0.1317	0.109*

Atomic displacement parameters ($\text{\AA}^2$)

	<i>U11</i>	<i>U22</i>	<i>U33</i>	<i>U12</i>	<i>U13</i>	<i>U23</i>
Cl1	0.0721 (4)	0.0596 (4)	0.0661 (4)	0.0020 (3)	0.0352 (3)	−0.0003 (3)
S2	0.0520 (4)	0.0574 (4)	0.0488 (3)	0.0070 (3)	0.0094 (3)	0.0123 (3)
S3	0.0611 (4)	0.0544 (4)	0.0515 (4)	−0.0088 (3)	0.0010 (3)	0.0002 (3)
O4	0.0348 (8)	0.0687 (11)	0.0426 (8)	0.0033 (7)	−0.0037 (6)	−0.0018 (7)
O5	0.0339 (9)	0.1056 (16)	0.0615 (11)	0.0060 (9)	−0.0060 (8)	−0.0079 (10)
N6	0.0337 (10)	0.0779 (15)	0.0443 (10)	0.0001 (9)	0.0037 (8)	0.0131 (10)
C7	0.0482 (13)	0.0288 (10)	0.0512 (12)	−0.0003 (8)	0.0186 (10)	−0.0030 (8)
C8	0.0337 (11)	0.0403 (12)	0.0594 (14)	0.0004 (8)	0.0099 (9)	−0.0017 (9)
C9	0.0338 (11)	0.0408 (12)	0.0488 (12)	0.0012 (8)	0.0009 (8)	0.0020 (9)
C10	0.0328 (10)	0.0290 (10)	0.0430 (10)	0.0004 (7)	0.0031 (8)	−0.0025 (8)
C11	0.0338 (10)	0.0331 (10)	0.0437 (11)	0.0011 (8)	0.0028 (8)	−0.0037 (8)
C12	0.0510 (13)	0.0400 (12)	0.0420 (11)	0.0034 (9)	0.0051 (9)	−0.0024 (9)
C13	0.0316 (10)	0.0375 (11)	0.0414 (10)	0.0018 (8)	0.0017 (8)	−0.0002 (8)
C14	0.0341 (11)	0.0486 (12)	0.0435 (11)	−0.0003 (9)	0.0038 (8)	−0.0015 (9)



C15	0.0340 (11)	0.0522 (13)	0.0504 (13)	0.0018 (9)	0.0017 (9)	−0.0054 (10)
C16	0.0334 (11)	0.0749 (17)	0.0423 (12)	0.0060 (10)	0.0053 (9)	0.0067 (11)

C17	0.0290 (10)	0.0613 (14)	0.0333 (10)	−0.0022 (9)	−0.0049 (8)	0.0041 (9)
C18	0.0583 (17)	0.121 (3)	0.0559 (16)	0.0283 (17)	0.0194 (13)	0.0135 (16)
C19	0.0546 (17)	0.098 (2)	0.0648 (17)	−0.0167 (15)	0.0069 (13)	0.0295 (16)
Geometric parameters (Å, °)						
C11—C7		1.739 (2)		C10— C11	1.393 (3)	
S2—C17		1.783 (2)		C10— C13	1.454 (3)	
S2—C16		1.788 (2)		C11— C12	1.384 (3)	
S3—C17		1.662 (2)		C12— H12	0.93	
O4—C11		1.371 (2)		C13— C14	1.343 (3)	
O4—C15		1.376 (3)		C13— C16	1.499 (3)	
O5—C15		1.200 (3)		C14— C15	1.438 (3)	
N6—C17		1.329 (3)		C14— H14	0.93	
N6—C19		1.454 (4)		C16— H16A	0.97	
N6—C18		1.467 (4)		C16— H16B	0.97	
C7—C12		1.371 (3)		C18— H18A	0.96	
C7—C8		1.372 (3)		C18— H18B	0.96	
C8—C9		1.379 (3)		C18— H18C	0.96	
C8—H8		0.93		C19— H19A	0.96	
C9—C10		1.401 (3)		C19— H19B	0.96	
C9—H9		0.93		C19— H19C	0.96	
C17—S2—C16		104.01 (11)		C13—	118.4	



		C14—H14	
C11—O4—C15	121.85 (16)	C15— C14—H14	118.4
C17—N6—C19	124.2 (2)	O5— C15—O4	117.2 (2)
C17—N6—C18	120.2 (2)	O5— C15—C14	126.0 (2)
C19—N6—C18	115.5 (2)	O4— C15—C14	116.79 (18)
C12—C7—C8	122.1 (2)	C13— C16—S2	117.08 (16)
C12—C7—C11	117.81 (18)	C13— C16—H16A	108
C8—C7—C11	120.11 (17)	S2— C16—H16A	108
C7—C8—C9	118.96 (19)	C13— C16—H16B	108
C7—C8—H8	120.5	S2— C16—H16B	108
C9—C8—H8	120.5	H16A— C16—H16B	107.3
C8—C9—C10	121.6 (2)	N6— C17—S3	124.16 (19)
C8—C9—H9	119.2	N6— C17—S2	112.87 (18)
C10—C9—H9	119.2	S3— C17—S2	122.96 (12)
C11—C10—C9	116.91 (19)	N6— C18—H18A	109.5
C11—C10—C13	117.79 (17)	N6— C18—H18B	109.5
C9—C10—C13	125.30 (19)	H18A— C18—H18B	109.5
O4—C11—C12	116.00 (18)	N6— C18—H18C	109.5
O4—C11—C10	121.68 (18)	H18A— C18—H18C	109.5
C12—C11—C10	122.32 (19)	H18B— C18—H18C	109.5
C7—C12—C11	118.2 (2)	N6— C19—H19A	109.5
C7—C12—H12	120.9	N6— C19—H19B	109.5
C11—C12—H12	120.9	H19A— C19—H19B	109.5
C14—C13—C10	118.76 (18)	N6—	109.5



		C19—H19C	
C14—C13—C16	122.68 (18)	H19A— C19—H19C	109.5
C10—C13—C16	118.54 (17)	H19B— C19—H19C	109.5
C13—C14—C15	123.1 (2)		
C9 C12—C7—C8—	0.2 (4)	C11— C10—C13— C16	177.7 (2)
C11—C7—C8—C9	−179.18 (19)	C9— C10—C13— C16	−2.7 (4)
C10 C7—C8—C9—	0.0 (4)	C10— C13—C14— C15	1.1 (4)

C8—C9—C10—C11	−0.2 (4)		C16—C13—C14—C15		−177.2 (3)
C8—C9—C10—C13	−179.8 (2)		C11—O4—C15—O5		179.8 (2)
C15—O4—C11—C12	−179.5 (2)		C11—O4—C15—C14		−0.1 (4)
C15—O4—C11—C10	0.4 (3)		C13—C14—C15—O5		179.4 (3)
C9—C10—C11—O4	−179.7 (2)		C13—C14—C15—O4		−0.7 (4)
C13—C10—C11—O4	0.0 (3)		C14—C13—C16—S2		−20.1 (4)
C9—C10—C11—C12	0.2 (3)		C10—C13—C16—S2		161.62 (19)
C13—C10—C11—C12	179.9 (2)		C17—S2—C16—C13		85.7 (2)
C8—C7—C12—C11	−0.1 (4)		C19—N6—C17—S3		−180.0 (2)
C11—C7—C12—C11	179.23 (18)		C18—N6—C17—S3		−2.9 (3)
O4—C11—C12—C7	179.9 (2)		C19—N6—C17—S2		0.4 (3)
C10—C11—C12—C7	−0.1 (4)		C18—N6—C17—S2		177.4 (2)
C11—C10—C13—C14	−0.7 (3)		C16—S2—C17—N6		−176.84 (18)
C9—C10—C13—C14	178.9 (2)		C16—S2—C17—S3		3.46 (19)
<i>Hydrogen-bond geometry (Å, °)</i>					
<i>D—H⋯A</i>		<i>D—H</i>	<i>H⋯A</i>	<i>D⋯A</i>	<i>D—H⋯A</i>
C16—H16A⋯S3i		0.97	2.83	3.707 (2)	150
Symmetry code: (i) −x, y+1/2, −z+1/2.					