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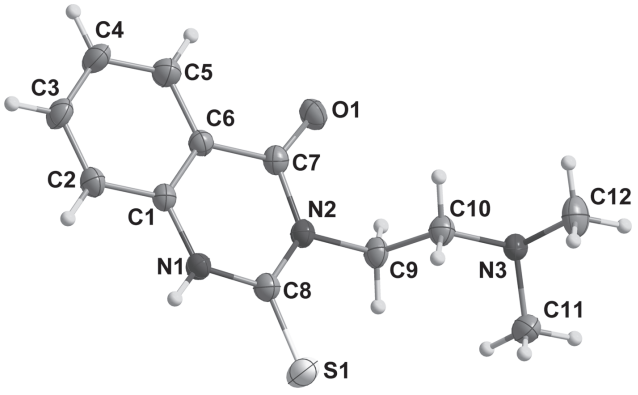
Crystal structure of 3-(2-dimethylaminoethyl)-2,3-dihydro-2-thioxoquinazolin-4(1*H*)-one, $C_{12}H_{15}N_3OS$



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Abstract

$C_{12}H_{15}N_3OS$, monoclinic, $P2_1/c$ (no. 14), $a = 7.9840(18)$ Å, $b = 11.331(3)$ Å, $c = 14.428(3)$ Å, $\beta = 105.702(4)°$, $V = 1256.5(5)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0639$, $wR_{ref}(F^2) = 0.1293$, $T = 296$K.

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The crystal asymmetric unit of the title structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was synthesized according to the literature known method [5]. The crystal suitable for single X-ray diffraction was obtained by recrystallization from acetonitrile solution at room temperature.

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Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	0.12 × 0.10 × 0.08 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.25 mm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω-scans
θ_{max}, completeness:	27.5°, >98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7350, 2832, 0.069
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1311
$N(param)_{refined}$:	155
Programs:	Bruker programs [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
S1	0.57030(15)	1.11873(11)	0.21409(9)	0.0687(4)
O1	0.9680(3)	0.8639(2)	0.45619(17)	0.0486(7)
C1	0.5051(4)	0.8952(3)	0.4105(2)	0.0359(9)
C2	0.3622(4)	0.8552(3)	0.4407(3)	0.0439(10)
H2A	0.250769	0.882373	0.410690	0.053*
C3	0.3882(5)	0.7765(3)	0.5141(3)	0.0516(11)
H3A	0.293725	0.750004	0.534457	0.062*
C4	0.5545(5)	0.7347(4)	0.5595(3)	0.0606(12)
H4A	0.570238	0.680870	0.609802	0.073*
C5	0.6945(5)	0.7729(3)	0.5301(3)	0.0523(11)
H5A	0.805280	0.744517	0.559890	0.063*
C6	0.6703(4)	0.8547(3)	0.4550(2)	0.0366(9)
C7	0.8196(5)	0.8984(3)	0.4233(3)	0.0396(9)
C8	0.6117(5)	1.0219(3)	0.3034(3)	0.0432(9)
C9	0.9268(4)	1.0319(3)	0.3199(3)	0.0417(9)
H9A	1.028302	1.034825	0.374970	0.050*
H9B	0.899959	1.111834	0.296570	0.050*
C10	0.9672(5)	0.9571(3)	0.2411(3)	0.0438(10)
H10A	0.989744	0.876615	0.263877	0.053*
H10B	0.866494	0.956267	0.185492	0.053*
C11	1.0824(5)	1.1182(4)	0.1667(3)	0.0652(13)
H11A	1.182797	1.145382	0.148492	0.098*
H11C	0.985274	1.112557	0.110582	0.098*
H11D	1.055376	1.172852	0.211464	0.098*
C12	1.1605(5)	0.9175(4)	0.1441(3)	0.0634(13)
H12C	1.259153	0.945675	0.124542	0.095*
H12D	1.187266	0.842046	0.174734	0.095*
H12A	1.062522	0.909863	0.088575	0.095*
N1	0.4818(4)	0.9755(3)	0.3365(2)	0.0420(8)
H1A	0.377211	0.997961	0.309111	0.050*
N2	0.7782(4)	0.9832(3)	0.3500(2)	0.0403(8)
N3	1.1185(4)	1.0018(2)	0.2121(2)	0.0399(8)

Experimental details

The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Discussion

Quinazoline derivatives have been paid much attention primarily due to their wide variety of pharmacological activities [4–6]. Our previous work report the structure of 3-methyl-2,3-dihydro-2-thioxoquinazolin-4(1*H*)-one [7]. As one of its structurally analogous, the structure of the title compound is presented in this paper.

In the title compound, the bond lengths are comparable with those found in our previous work [7]. In the crystal, intermolecular N—H· · · N hydrogen bonds link the molecules into one dimentional chains along *a* axis.

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