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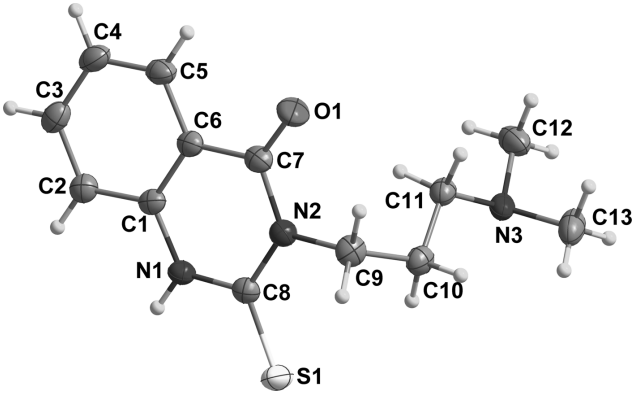
Crystal structure of 3-(3-dimethylaminopropyl)-2,3-dihydro-2-thioxoquinazolin-4(1*H*)-one, $C_{13}H_{17}N_3OS$



https://doi.org/10.1515/ncrs-2017-0203
Received October 14, 2017; accepted November 25, 2017; available online December 16, 2017

Abstract

$C_{13}H_{17}N_3OS$, monoclinic, $P2_1/c$ (no. 14), $a = 9.3721(9)$ Å, $b = 15.3783(14)$ Å, $c = 9.1684(9)$ Å, $\beta = 96.698(2)°$, $V = 1312.4(2)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0371$, $wR_{ref}(F^2) = 0.0826$, $T = 296$ K.

CCDC no.: 1587582

Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	0.16 × 0.15 × 0.13 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.24 mm^{-1}
Diffractometer, scan mode:	CCD area detector φ and ω-scans
θ_{max}, completeness:	27.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7855, 2980, 0.023
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2259
$N(param)_{refined}$:	166
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	0.07009(5)	0.10208(3)	0.34148(5)	0.05670(15)
O1	0.34313(13)	0.09853(8)	0.83937(12)	0.0617(3)
N1	0.25681(12)	−0.01528(8)	0.44693(13)	0.0387(3)
H1A	0.239607	−0.038524	0.361371	0.046*
N2	0.21947(12)	0.09631(8)	0.60980(13)	0.0385(3)
N3	−0.17075(13)	0.10887(9)	0.82569(14)	0.0465(3)
C1	0.35413(14)	−0.05643(9)	0.54872(15)	0.0365(3)
C2	0.42504(16)	−0.13200(10)	0.51235(18)	0.0447(4)
H2A	0.407333	−0.155375	0.418431	0.054*
C3	0.52112(17)	−0.17150(11)	0.6164(2)	0.0517(4)
H3A	0.568438	−0.221698	0.592227	0.062*
C4	0.54852(17)	−0.13748(12)	0.7572(2)	0.0564(4)
H4A	0.612837	−0.165151	0.827115	0.068*
C5	0.48035(16)	−0.06301(12)	0.79260(17)	0.0506(4)
H5A	0.498752	−0.040101	0.886798	0.061*
C6	0.38318(14)	−0.02103(10)	0.68818(16)	0.0396(3)
C7	0.31673(15)	0.06085(10)	0.72224(16)	0.0428(3)
C8	0.18701(15)	0.05862(9)	0.47217(16)	0.0389(3)
C9	0.15533(17)	0.18161(9)	0.63925(18)	0.0478(4)
H9A	0.159018	0.218666	0.554156	0.057*
H9B	0.213236	0.208747	0.721415	0.057*
C10	0.00138(17)	0.17670(10)	0.67355(18)	0.0470(4)
H10A	−0.033938	0.235337	0.684689	0.056*
H10B	−0.056817	0.150379	0.590756	0.056*
C11	−0.01826(15)	0.12554(10)	0.81037(17)	0.0452(4)
H11A	0.031728	0.070439	0.807565	0.054*
H11B	0.024736	0.157414	0.895679	0.054*
C12	−0.18215(19)	0.04915(14)	0.94797(19)	0.0646(5)
H12A	−0.137344	−0.005151	0.928813	0.097*
H12B	−0.281613	0.039414	0.958474	0.097*
H12C	−0.134967	0.073981	1.036863	0.097*
C13	−0.2473(2)	0.18967(14)	0.8510(2)	0.0724(6)
H13A	−0.242958	0.228214	0.769320	0.109*
H13B	−0.203181	0.216974	0.939139	0.109*
H13C	−0.345825	0.176703	0.861290	0.109*

The crystal 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 a literature known method [5]. The crystal suitable for single X-ray

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diffraction was obtained by recrystallization from acetonitrile solution at room temperature.

Experimental details

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

Discussion

Quinazoline derivatives exhibit a wide variety of pharmacological activities [4–6], and they are important intermediates in the synthesis of a variety of valuable heterocyclic compounds [5]. In fact, the structure of 3-methyl-2,3-dihydro-2-thioxoquinazolin-4(1*H*)-one has been demonstrated in our previous work [7]. As one of its structurally analogous, the title compound is reported here.

In the title compound, the bond lengths are comparable with those found in the literature [7]. In the crystal, pairs of intermolecular N—H· · · N hydrogen bonds link two molecules into a centrosymmetric dimer.

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