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1-Propyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide

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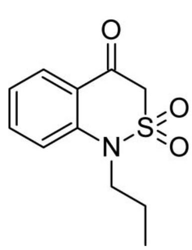
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.111; data-to-parameter ratio = 18.9.

In the title compound, $C_{11}H_{13}NO_3S$, a benzothiazine derivative, the heterocycle adopts a sofa conformation. In the crystal, weak C—H⋯O hydrogen bonds connect the molecules into a three-dimensional network.

Related literature

For the synthesis of the title compound, see: Volovenko *et al.* (2007). For a related structure, see: Shafiq *et al.* (2009).



Experimental

Crystal data

$C_{11}H_{13}NO_3S$
M_r = 239.28
Triclinic, $P\bar{1}$
a = 7.9448 (2) Å
b = 8.0701 (3) Å
c = 9.6267 (2) Å
α = 87.468 (2)°
β = 84.097 (2)°
γ = 64.453 (1)°
V = 553.92 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 296 K
0.28 × 0.21 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.925, T_{max} = 0.967
12058 measured reflections
2765 independent reflections
2229 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.111
S = 1.07
2765 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C11—H11B⋯O2^{i}	0.96	2.57	3.346 (2)	138
C8—H8A⋯O3^{ii}	0.97	2.55	3.453 (2)	155
C2—H2⋯O1^{iii}	0.93	2.55	3.4665 (19)	170

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5369).

References

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supporting information

Acta Cryst. (2010). E**66**, o2839 [https://doi.org/10.1107/S160053681004078X]

1-Propyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide

Islam Ullah Khan, Muhammad Shafiq and Muhammad Nadeem Arshad

S1. Comment

Here we report the crystal structure of title compound in countinuation to the previously published 3,3-dichloro-1-ethyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide derivative (Shafiq *et al.*, 2009). The difference between the two compounds is a propyl which differ just only in substitution at N and at the methylene C atom in the benzothiazine ring. The heterocycle adopts a sofa conformation. Weak C—H···O type hydrogen bonds connect the molecules to a three dimensional network.

S2. Experimental

The title compound was prepared following the available literature procedure (Volovenko *et al.*, 2007).

S3. Refinement

All the C—H H-atoms were positioned with idealized geometry with C—H = 0.93 Å for aromatic C—H = 0.97 Å for methylene C—H = 0.96 Å for methyl and were refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C) for aromatic, with U_{iso}(H) = 1.2 U_{eq}(C) for methylene, with U_{iso}(H) = 1.5 U_{eq}(C) for methyl.

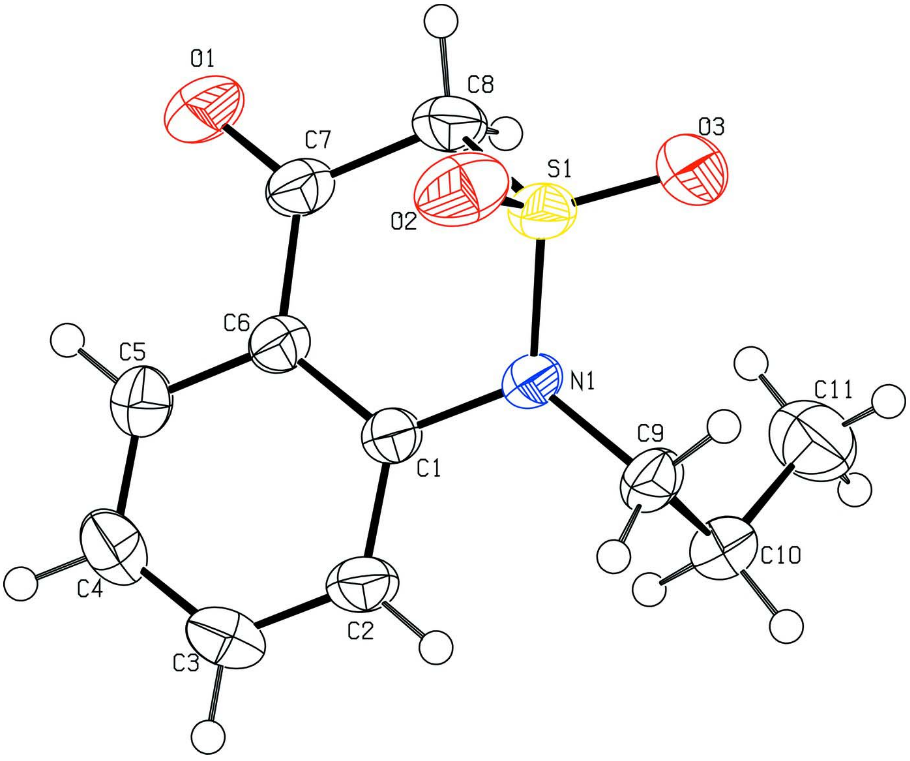

Figure 1

Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

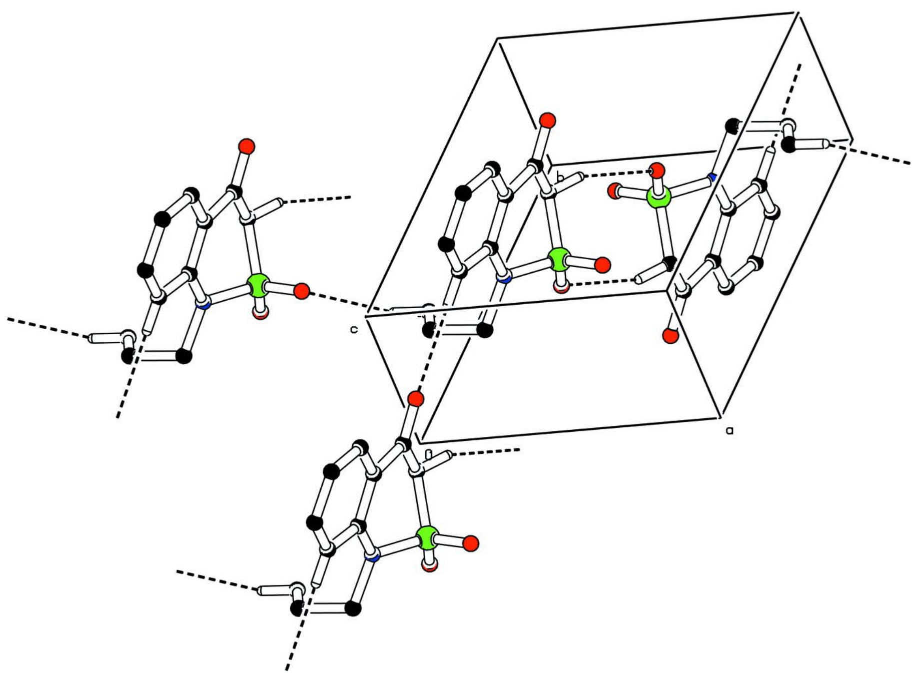

Figure 2

Unit cell packing diagram showing the hydrogen bonding with dashed lines.

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Crystal data

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M_r = 239.28
Triclinic, $P\overline{1}$
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a = 7.9448 (2) Å
b = 8.0701 (3) Å
c = 9.6267 (2) Å
α = 87.468 (2)°
β = 84.097 (2)°
γ = 64.453 (1)°
V = 553.92 (2) Å^3
Z = 2
F(000) = 252
D_x = 1.435 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5097 reflections
θ = 2.2–21.8°
μ = 0.28 mm^{-1}
T = 296 K
Needle, light brown
0.28 × 0.21 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.925, T_{max} = 0.967
12058 measured reflections
2765 independent reflections
2229 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 28.3°, θ_{min} = 2.1°
h = −10→10
k = −10→10
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.111
S = 1.07
2765 reflections
146 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.0882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	0.44648 (6)	0.31465 (5)	0.66978 (4)	0.04181 (14)
O1	0.2757 (2)	0.71661 (17)	0.91660 (14)	0.0633 (4)
O2	0.62535 (17)	0.25460 (17)	0.71992 (15)	0.0584 (3)

O3	0.4391 (2)	0.2879 (2)	0.52525 (12)	0.0680 (4)
N1	0.31827 (18)	0.22605 (17)	0.76115 (12)	0.0380 (3)
C1	0.28023 (19)	0.26527 (18)	0.90617 (14)	0.0313 (3)
C2	0.2496 (2)	0.1412 (2)	0.99954 (16)	0.0408 (3)
H2	0.2519	0.0338	0.9661	0.049*
C3	0.2161 (2)	0.1770 (2)	1.14058 (16)	0.0473 (4)
H3	0.1951	0.0935	1.2012	0.057*
C4	0.2129 (2)	0.3344 (2)	1.19393 (17)	0.0494 (4)
H4	0.1947	0.3549	1.2898	0.059*
C5	0.2372 (2)	0.4602 (2)	1.10331 (16)	0.0421 (3)
H5	0.2322	0.5679	1.1384	0.051*
C6	0.26911 (19)	0.42939 (18)	0.95988 (14)	0.0323 (3)
C7	0.2874 (2)	0.57493 (19)	0.87064 (16)	0.0376 (3)
C8	0.3163 (3)	0.5469 (2)	0.71447 (16)	0.0447 (4)
H8A	0.3812	0.6171	0.6723	0.054*
H8B	0.1953	0.5924	0.6773	0.054*
C9	0.3171 (2)	0.0585 (2)	0.70536 (16)	0.0398 (3)
H9A	0.3717	−0.0425	0.7696	0.048*
H9B	0.3936	0.0264	0.6168	0.048*
C10	0.1214 (2)	0.0854 (2)	0.68464 (17)	0.0461 (4)
H10A	0.0411	0.1345	0.7699	0.055*
H10B	0.1236	−0.0331	0.6673	0.055*
C11	0.0384 (3)	0.2133 (3)	0.5651 (2)	0.0662 (5)
H11A	0.0339	0.3315	0.5821	0.099*
H11B	−0.0860	0.2258	0.5575	0.099*
H11C	0.1149	0.1637	0.4797	0.099*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0535 (3)	0.0410 (2)	0.0377 (2)	−0.02944 (19)	0.01063 (16)	−0.00505 (15)
O1	0.0991 (11)	0.0410 (7)	0.0630 (8)	−0.0439 (7)	0.0020 (7)	−0.0069 (6)
O2	0.0442 (7)	0.0516 (7)	0.0801 (9)	−0.0240 (6)	0.0097 (6)	−0.0051 (6)
O3	0.1086 (11)	0.0773 (9)	0.0367 (7)	−0.0615 (9)	0.0177 (7)	−0.0119 (6)
N1	0.0526 (7)	0.0369 (6)	0.0339 (6)	−0.0295 (6)	0.0055 (5)	−0.0063 (5)
C1	0.0338 (7)	0.0295 (7)	0.0321 (7)	−0.0157 (5)	−0.0007 (5)	−0.0004 (5)
C2	0.0499 (9)	0.0319 (7)	0.0438 (8)	−0.0219 (7)	0.0001 (6)	0.0035 (6)
C3	0.0532 (10)	0.0467 (9)	0.0407 (9)	−0.0222 (8)	−0.0008 (7)	0.0127 (7)
C4	0.0580 (10)	0.0567 (10)	0.0307 (7)	−0.0227 (8)	−0.0012 (7)	0.0008 (7)
C5	0.0479 (9)	0.0413 (8)	0.0382 (8)	−0.0201 (7)	−0.0012 (6)	−0.0070 (6)
C6	0.0338 (7)	0.0294 (7)	0.0353 (7)	−0.0151 (5)	−0.0021 (5)	−0.0008 (5)
C7	0.0419 (8)	0.0297 (7)	0.0438 (8)	−0.0184 (6)	−0.0010 (6)	−0.0004 (6)
C8	0.0595 (10)	0.0351 (8)	0.0426 (8)	−0.0249 (7)	0.0003 (7)	0.0064 (6)
C9	0.0488 (9)	0.0321 (7)	0.0419 (8)	−0.0211 (6)	0.0016 (6)	−0.0089 (6)
C10	0.0573 (10)	0.0497 (9)	0.0436 (8)	−0.0347 (8)	−0.0039 (7)	−0.0002 (7)
C11	0.0646 (12)	0.0862 (15)	0.0562 (11)	−0.0401 (11)	−0.0128 (9)	0.0161 (10)

Geometric parameters (Å, º)

S1—O2	1.4191 (14)	C5—C6	1.3915 (19)
S1—O3	1.4282 (13)	C5—H5	0.9300
S1—N1	1.6464 (12)	C6—C7	1.473 (2)
S1—C8	1.7535 (16)	C7—C8	1.509 (2)
O1—C7	1.2069 (18)	C8—H8A	0.9700
N1—C1	1.4178 (17)	C8—H8B	0.9700
N1—C9	1.4808 (17)	C9—C10	1.508 (2)
C1—C2	1.3982 (19)	C9—H9A	0.9700
C1—C6	1.4070 (18)	C9—H9B	0.9700
C2—C3	1.375 (2)	C10—C11	1.513 (3)
C2—H2	0.9300	C10—H10A	0.9700
C3—C4	1.380 (2)	C10—H10B	0.9700
C3—H3	0.9300	C11—H11A	0.9600
C4—C5	1.373 (2)	C11—H11B	0.9600
C4—H4	0.9300	C11—H11C	0.9600
O2—S1—O3	117.98 (9)	O1—C7—C6	122.99 (14)
O2—S1—N1	111.54 (7)	O1—C7—C8	118.84 (13)
O3—S1—N1	107.86 (7)	C6—C7—C8	118.14 (12)
O2—S1—C8	107.87 (8)	C7—C8—S1	111.75 (10)
O3—S1—C8	110.27 (9)	C7—C8—H8A	109.3
N1—S1—C8	99.80 (7)	S1—C8—H8A	109.3
C1—N1—C9	120.81 (11)	C7—C8—H8B	109.3
C1—N1—S1	116.96 (9)	S1—C8—H8B	109.3
C9—N1—S1	117.37 (10)	H8A—C8—H8B	107.9
C2—C1—C6	118.28 (13)	N1—C9—C10	111.75 (13)
C2—C1—N1	120.18 (12)	N1—C9—H9A	109.3
C6—C1—N1	121.53 (12)	C10—C9—H9A	109.3
C3—C2—C1	120.42 (14)	N1—C9—H9B	109.3
C3—C2—H2	119.8	C10—C9—H9B	109.3
C1—C2—H2	119.8	H9A—C9—H9B	107.9
C2—C3—C4	121.32 (14)	C9—C10—C11	113.28 (15)
C2—C3—H3	119.3	C9—C10—H10A	108.9
C4—C3—H3	119.3	C11—C10—H10A	108.9
C5—C4—C3	118.96 (14)	C9—C10—H10B	108.9
C5—C4—H4	120.5	C11—C10—H10B	108.9
C3—C4—H4	120.5	H10A—C10—H10B	107.7
C4—C5—C6	121.20 (14)	C10—C11—H11A	109.5
C4—C5—H5	119.4	C10—C11—H11B	109.5
C6—C5—H5	119.4	H11A—C11—H11B	109.5
C5—C6—C1	119.74 (13)	C10—C11—H11C	109.5
C5—C6—C7	117.26 (12)	H11A—C11—H11C	109.5
C1—C6—C7	122.99 (12)	H11B—C11—H11C	109.5
O2—S1—N1—C1	59.41 (12)	C2—C1—C6—C5	3.0 (2)
O3—S1—N1—C1	−169.51 (11)	N1—C1—C6—C5	−178.04 (13)

C8—S1—N1—C1	−54.35 (12)	C2—C1—C6—C7	−176.18 (14)
O2—S1—N1—C9	−96.15 (12)	N1—C1—C6—C7	2.8 (2)
O3—S1—N1—C9	34.93 (14)	C5—C6—C7—O1	−0.1 (2)
C8—S1—N1—C9	150.09 (12)	C1—C6—C7—O1	179.13 (15)
C9—N1—C1—C2	3.0 (2)	C5—C6—C7—C8	−178.19 (13)
S1—N1—C1—C2	−151.64 (12)	C1—C6—C7—C8	1.0 (2)
C9—N1—C1—C6	−175.92 (13)	O1—C7—C8—S1	148.80 (14)
S1—N1—C1—C6	29.41 (17)	C6—C7—C8—S1	−32.99 (17)
C6—C1—C2—C3	−2.2 (2)	O2—S1—C8—C7	−61.58 (13)
N1—C1—C2—C3	178.80 (14)	O3—S1—C8—C7	168.29 (11)
C1—C2—C3—C4	−0.5 (2)	N1—S1—C8—C7	54.98 (12)
C2—C3—C4—C5	2.4 (3)	C1—N1—C9—C10	82.62 (17)
C3—C4—C5—C6	−1.6 (3)	S1—N1—C9—C10	−122.81 (12)
C4—C5—C6—C1	−1.1 (2)	N1—C9—C10—C11	70.53 (19)
C4—C5—C6—C7	178.08 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*B*···O2^{i}	0.96	2.57	3.346 (2)	138
C8—H8*A*···O3^{ii}	0.97	2.55	3.453 (2)	155
C2—H2···O1^{iii}	0.93	2.55	3.4665 (19)	170

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*.