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Methyl 2-benzyl-4-hydroxy-1,1-dioxo-1,2,3,4-tetrahydro-1λ^6,2-benzothiazine-3-carboxylate

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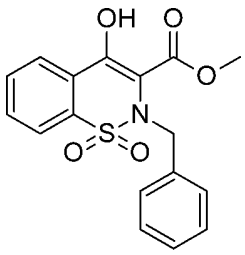
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.119; data-to-parameter ratio = 16.8.

In the title compound, $C_{17}H_{15}NO_5S$, the benzene ring of the fused-ring system is twisted by 11.67 (6)° with respect to the thiazine ring. The atoms of the four-atom methyl ester group and the phenyl ring of the benzyl unit are inclined at 16.50 (7) and 44.52 (3)° with respect to the thiazine ring. An intramolecular O—H···O hydrogen bond gives rise to a six-membered S(6) ring motif. In the crystal, molecules are extended through a C—H···O interaction along the a axis. C—H···π interactions are also observed.

Related literature

For the biological properties of benzothiazines, see: Zia-ur-Rehman *et al.* (2005, 2006). For a related structure, see: Arshad *et al.* (2009). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{15}NO_5S$
M_r = 345.36
Monoclinic, $P2_1/c$
a = 9.4920 (15) Å
b = 10.9607 (17) Å
c = 15.050 (2) Å
β = 99.758 (2)°
V = 1543.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 173 K
0.43 × 0.25 × 0.19 mm

Data collection

Bruker SMART 1K diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.905, T_{max} = 0.956
13430 measured reflections
3719 independent reflections
3297 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.119
S = 1.06
3719 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O4^{i}	0.95	2.49	3.1861 (19)	130
O1—H1*O*···O4	0.93 (2)	1.72 (2)	2.5580 (15)	149 (2)
C10—H10*B*···*Cg*1^{ii}	0.80	2.94	3.6391 (18)	130

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

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 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *X-SEED* (Barbour, 2001), *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5172).

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