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2-[2-(2-Bromophenyl)-2-oxoethyl]-1λ^6,2-benzothiazole-1,1,3-trione

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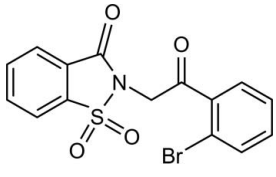
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.105; data-to-parameter ratio = 16.5.

The asymmetric unit of the title compound, $C_{15}H_{10}BrNO_4S$, contains two different conformers in which the benzisothiazole rings are essentially planar, with r.m.s. deviations of 0.012 and 0.017 Å. The mean planes of the benzene rings form dihedral angles 70.49 (13) and 72.79 (11)° with the benzisothiazole rings. The orientation of the Br atoms in the two conformers exhibit the most pronounced difference, with opposing orientations in the two molecules. The crystal structure is stabilized by π–π interactions between the benzene rings of the benzisothiazole moieties of one molecule and bromobenzene rings of the other molecule, with distances between the ring centroids of 3.599 (3) and 3.620 (3) Å, respectively. The crystal packing is further consolidated by pairs of weak intermolecular C—H···O hydrogen bonds, which form inversion dimers.

Related literature

For non-steroidal anti-inflammatory drugs (NSAIDs) and related compounds, see: Lombardino *et al.* (1971); Soler (1985); Carty *et al.* (1993); Turck *et al.* (1995); Blackham & Owen (1975); Singh *et al.* (2007); Vaccarino *et al.* (2007); Kapui *et al.* (2003). For related structures, see: Maliha *et al.* (2007); Siddiqui *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{10}BrNO_4S$
M_r = 380.21
Triclinic, $P\overline{1}$
a = 7.574 (2) Å
b = 13.903 (4) Å
c = 14.814 (4) Å
α = 110.574 (15)°
β = 96.936 (13)°
γ = 93.640 (14)°
V = 1440.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.02 mm^{-1}
T = 123 K
0.18 × 0.18 × 0.16 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.613, T_{max} = 0.644
12284 measured reflections
6541 independent reflections
5268 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.105
S = 1.12
6541 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O1^{i}	0.95	2.40	3.305 (5)	159
C17—H17···O5^{ii}	0.95	2.43	3.225 (5)	141
C27—H27···O7^{iii}	0.95	2.29	3.164 (5)	153

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y, -z+1$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); 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); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2412).

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