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2-Chloro-4-(2-iodobenzenesulfonamido)-benzoic acid

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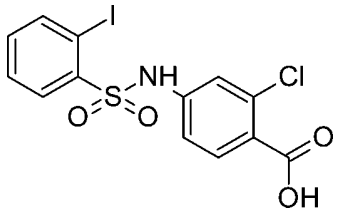
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.010 Å; R factor = 0.054; wR factor = 0.129; data-to-parameter ratio = 19.2.

In the title compound, $C_{13}H_9ClINO_4S$, the dihedral angle between the aromatic rings is 81.04 (17)°. The disposition of the I and Cl atoms attached to the two rings is *anti*. In the crystal, molecules are connected *via* O—H···O and N—H···O hydrogen bonds.

Related literature

For background to thiazine heterocycles, see: Arshad *et al.* (2008, 2011). For their biological activity, see: Medina *et al.* (1999). For related structures, see: Arshad *et al.* (2009*a*,*b*,*c*).



Experimental

Crystal data

$C_{13}H_9ClINO_4S$
M_r = 437.62
Monoclinic, $P2_1/n$
a = 14.1522 (8) Å
b = 7.3203 (4) Å
c = 14.7193 (8) Å
β = 104.892 (2)°
V = 1473.68 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.51 mm^{-1}
T = 296 K
0.18 × 0.15 × 0.09 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.661, T_{max} = 0.806
16645 measured reflections
3668 independent reflections
1876 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.129
S = 1.03
3668 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.24 e Å^{-3}
$\Delta\rho_{min}$ = −1.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.38	3.214 (6)	162
O1—H1O···O2^{ii}	0.82	2.09	2.771 (6)	140

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

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* (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: HB5865).

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