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4-Bromo-2-((*E*)-{4-[(3,4-dimethylisoxazol-5-yl)sulfamoyl]phenyl}iminiomethyl)phenolate

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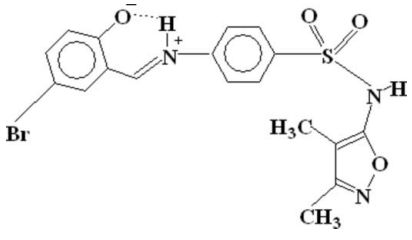
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.116; data-to-parameter ratio = 15.7.

The title compound, $C_{18}H_{16}BrN_3O_4S$, is a Schiff base ligand of 5-bromosalicylaldehyde and sulfisoxazole [or *N*-(3,4-dimethyl-5-isoxazol)sulfanilamide]. The present structure is a zwitterion and is a more precise reinterpretation of the structure which was originally reported by Hämäläinen, Lehtinen & Turpeinen [*Arch. Pharm.* (1986), **319**, 415–420]. The two aromatic rings which make π–π interactions [centroid–centroid distance 3.7538 (18) Å] through intermolecular interactions. There is also a C—Br$\cdots\pi$ interaction [3.6333 (15) Å] with the heterocyclic ring. An intramolecular N—H$\cdots$O hydrogen bond also exists. Dimers are formed due to intermolecular N—H$\cdots$O hydrogen bonding. Intermolecular C—H$\cdots$O hydrogen bonding links a methyl C atom and the phenolate O atom. The dimers are linked by C—H$\cdots$N hydrogen bonds, where the C atom is from the Schiff base group and the N atom is of five-membered heterocyclic ring.

Related literature

For related literature, see: Chohan *et al.* (2008); Hämäläinen *et al.* (1986); Shad *et al.* (2008).



Experimental

Crystal data

$C_{18}H_{16}BrN_3O_4S$
M_r = 450.31
Monoclinic, $P2_1/n$
a = 15.3846 (10) Å
b = 7.2235 (5) Å
c = 16.5520 (11) Å
β = 93.201 (4)°
V = 1836.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation radiation
μ = 2.38 mm^{-1}
T = 296 (2) K
0.18 × 0.14 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.685, T_{max} = 0.793
18874 measured reflections
3955 independent reflections
2704 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.00
3955 reflections
252 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O1	0.80 (3)	1.91 (3)	2.577 (4)	141 (3)
N2—H2$\cdots$O1^{i}	0.75 (3)	2.09	2.828 (4)	171 (4)
C17—H17*C*$\cdots$O1^{i}	0.96	2.58	3.248 (5)	126
C7—H7$\cdots$N3^{ii}	0.93	2.53	3.420 (4)	161

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2007); 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, 2003); 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: BQ2069).

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