

2-Bromo-1,2-diphenylethenyl 4-methylphenyl sulfoxide

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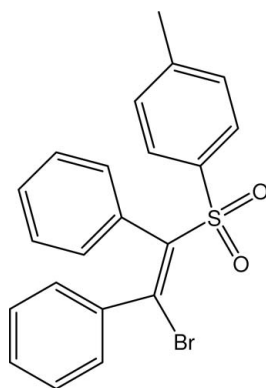
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Key indicators: single-crystal X-ray study; $T = 300$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.042; wR factor = 0.109; data-to-parameter ratio = 18.8.

In the title compound, $\text{C}_{21}\text{H}_{17}\text{BrO}_2\text{S}$, the two phenyl rings attached to the ethene group are oriented at dihedral angles of 76.19 (10) and 57.99 (8)° with respect to the $\text{Br}-\text{C}=\text{C}-\text{S}$ plane [r.m.s. deviation 0.003 Å]. The sulfonyl-bound phenyl ring forms a dihedral angle of 83.26 (8)° with the above plane. The crystal structure is stabilized by weak $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For the antibacterial activity of sulfone compounds, see: Mandell & Sande (1985). For a related structure, see: Wolf (1999). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{17}\text{BrO}_2\text{S}$	$V = 3725$ (3) Å ³
$M_r = 413.32$	$Z = 8$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 21.561$ (9) Å	$\mu = 2.33$ mm ⁻¹
$b = 8.505$ (4) Å	$T = 300$ K
$c = 21.134$ (10) Å	$0.15 \times 0.12 \times 0.08$ mm
$\beta = 106.044$ (9)°	

Data collection

Bruker SMART CCD area-detector diffractometer	12736 measured reflections
Absorption correction: multi-scan (SADABS, Bruker, 2001)	4273 independent reflections
$T_{\min} = 0.661$, $T_{\max} = 0.820$	2826 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	227 parameters
$wR(F^2) = 0.109$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.58$ e Å ⁻³
4273 reflections	$\Delta\rho_{\text{min}} = -0.30$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C12}-\text{H12}\cdots\text{Cg1}^{\text{i}}$	0.93	2.91	3.608 (5)	133
$\text{C19}-\text{H19}\cdots\text{Cg1}^{\text{ii}}$	0.93	2.88	3.786 (4)	166

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$. Cg1 is the centroid of the C3-C8 ring.

Data collection: *SMART* (Bruker 2001); cell refinement: *SAINT* (Bruker 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004), *PARST* (Nardelli, 1995) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2936).

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supplementary materials

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Comment

Sulfone compounds, similar to sulfonamides, show strong *in vitro* and *in vivo* antibacterial activity, and for almost 60 years they have been used successfully in medicine (Mandell & Sande, 1985). Certain sulfones also exhibit fungicidal activity.

The separation of the Br and S1 atoms [3.371 (2) Å] is less than the sum of their respective van der Waals radii 3.65 Å. Shortening of this interatomic distance has often been observed in α,α -unsubstituted β -ketosulfones and is usually explained by hyperconjugative cross-interaction involving the π^* (C2—Br)— σ (S1—C1) and π (C2—Br)— σ^* (S1—C1) pairs of bonding and non-bonding molecular orbitals. According to general theory of the anomeric effect, the largest overlapping of these orbitals should occur when the interacting polar bonds are situated in the *gauche* position. However, in the title compound, the S1—C1 and C2—Br bonds are almost planar [the S1—C1—C2—Br torsion angle is 0.9 (3)°]. The only existing *gauche* interactions involve S1O1 with the C1—C2 and C1—C9 bonds. In addition, the O1...C9 non-bonding distance [3.827 (2) Å] is much longer than the sum of the respective van der Waals radii (3.22 Å). Therefore, the main electronic interaction, despite the unfavoured planar arrangement, should be the Coulombic type, weak electronic interaction of the negatively charged bromine atom and the highly positive S atom, that is responsible for the electron-density transfer from the sulfonyl group towards the bromine atom. All the above features are similar to those reported for 4'-{[benzoyl(4-tolylhydrazono)methyl]sulfonyl}acetanilide (Wolf, 1999, and references therein). The bond lengths are consistent with values reported by Allen *et al.* (1987), and indicate high level of electron-density delocalization which exists in the planar phenyl rings attached to the ethene group.

Experimental

cis-Stilbene (4 g) was reacted with bromine (5 g) at 283 K to obtain dibromostilbene. The resultant compound was refluxed with paramethylphenyl sodium sulphonate (4.5 g) for 6 h. The reaction mixture was condensed to yield 5 mg of the title compound and was recrystallized from methanol.

Refinement

H-atoms were positioned at calculated positions [C—H = 0.93 Å (aromatic) and 0.96 Å (methyl)] and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}_{\text{aromatic}})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$.

Figures

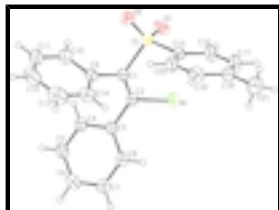


Fig. 1. The molecular structure of the title compound, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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Crystal data

$C_{21}H_{17}BrO_2S$

$M_r = 413.32$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 21.561 (9) \text{ \AA}$

$b = 8.505 (4) \text{ \AA}$

$c = 21.134 (10) \text{ \AA}$

$\beta = 106.044 (9)^\circ$

$V = 3725 (3) \text{ \AA}^3$

$Z = 8$

$F_{000} = 1680$

$D_x = 1.474 \text{ Mg m}^{-3}$

$D_m = 1.48 \text{ Mg m}^{-3}$

D_m measured by not measured

Melting point: 500 K

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4223 reflections

$\theta = 2-25^\circ$

$\mu = 2.33 \text{ mm}^{-1}$

$T = 300 \text{ K}$

Plate, colourless

$0.15 \times 0.12 \times 0.08 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 300 \text{ K}$

ω scans

Absorption correction: multi-scan (SADABS, Bruker, 2001)

$T_{\min} = 0.661$, $T_{\max} = 0.820$

12736 measured reflections

4273 independent reflections

2826 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 28.6^\circ$

$\theta_{\min} = 2.0^\circ$

$h = -28 \rightarrow 27$

$k = -11 \rightarrow 11$

$l = -28 \rightarrow 28$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.109$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.01$	$(\Delta/\sigma)_{\max} = 0.008$
4273 reflections	$\Delta\rho_{\max} = 0.58 \text{ e } \text{\AA}^{-3}$
227 parameters	$\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.11848 (11)	0.3985 (3)	0.54204 (12)	0.0459 (6)
C9	0.09957 (13)	0.2624 (3)	0.49692 (13)	0.0500 (6)
C3	0.12159 (11)	0.5778 (3)	0.44958 (12)	0.0440 (6)
C2	0.12993 (11)	0.5387 (3)	0.51983 (12)	0.0458 (6)
C4	0.06193 (13)	0.5579 (3)	0.40419 (13)	0.0514 (6)
H4	0.0273	0.5194	0.4177	0.062*
C6	0.10397 (15)	0.6526 (4)	0.31844 (14)	0.0645 (8)
H6	0.0981	0.6782	0.2744	0.077*
C10	0.03670 (16)	0.2091 (4)	0.47825 (15)	0.0657 (8)
H10	0.0056	0.2583	0.4943	0.079*
C8	0.17237 (13)	0.6357 (3)	0.42858 (14)	0.0534 (7)
H8	0.2126	0.6497	0.4586	0.064*
C13	0.1272 (3)	0.0614 (5)	0.4310 (2)	0.0968 (13)
H13	0.1579	0.0117	0.4146	0.116*
C7	0.16352 (16)	0.6726 (4)	0.36342 (15)	0.0635 (8)
H7	0.1979	0.7113	0.3495	0.076*
C5	0.05398 (13)	0.5952 (4)	0.33917 (14)	0.0606 (7)
H5	0.0139	0.5811	0.3089	0.073*
C14	0.14498 (17)	0.1862 (4)	0.47292 (17)	0.0698 (9)
H14	0.1877	0.2198	0.4853	0.084*
C12	0.0654 (3)	0.0094 (5)	0.41319 (19)	0.1024 (14)
H12	0.0542	-0.0770	0.3854	0.123*
C11	0.0197 (2)	0.0831 (4)	0.43584 (18)	0.0896 (12)
H11	-0.0229	0.0487	0.4228	0.108*
S1	0.12699 (3)	0.35497 (10)	0.62701 (3)	0.0549 (2)
O2	0.10422 (10)	0.1974 (3)	0.62829 (10)	0.0762 (7)
O1	0.09830 (8)	0.4768 (3)	0.65579 (9)	0.0712 (6)

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C15	0.21083 (12)	0.3535 (3)	0.66457 (12)	0.0480 (6)
C19	0.31330 (15)	0.2364 (4)	0.67791 (16)	0.0632 (8)
H19	0.3388	0.1601	0.6659	0.076*
C20	0.24851 (14)	0.2377 (3)	0.64798 (15)	0.0574 (7)
H20	0.2300	0.1617	0.6169	0.069*
C18	0.34187 (13)	0.3447 (4)	0.72521 (15)	0.0608 (7)
C16	0.23801 (13)	0.4638 (4)	0.71088 (13)	0.0614 (7)
H16	0.2127	0.5421	0.7219	0.074*
C17	0.30353 (14)	0.4575 (4)	0.74120 (15)	0.0695 (8)
H17	0.3220	0.5316	0.7732	0.083*
C21	0.41371 (15)	0.3392 (5)	0.7578 (2)	0.0926 (12)
H21A	0.4274	0.4369	0.7801	0.139*
H21B	0.4362	0.3226	0.7250	0.139*
H21C	0.4232	0.2546	0.7891	0.139*
Br	0.158444 (16)	0.71426 (4)	0.575988 (15)	0.07199 (15)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0358 (12)	0.0608 (16)	0.0377 (14)	-0.0047 (11)	0.0045 (11)	0.0023 (12)
C9	0.0575 (16)	0.0513 (15)	0.0386 (15)	-0.0036 (12)	0.0089 (13)	0.0057 (11)
C3	0.0453 (14)	0.0448 (13)	0.0384 (14)	-0.0040 (11)	0.0057 (11)	-0.0029 (11)
C2	0.0351 (12)	0.0582 (16)	0.0393 (14)	-0.0076 (11)	0.0025 (11)	-0.0033 (12)
C4	0.0445 (14)	0.0641 (17)	0.0430 (15)	-0.0024 (12)	0.0077 (12)	0.0001 (13)
C6	0.076 (2)	0.0751 (19)	0.0416 (16)	0.0031 (16)	0.0147 (16)	0.0003 (14)
C10	0.070 (2)	0.0679 (19)	0.0540 (19)	-0.0146 (16)	0.0086 (16)	-0.0039 (15)
C8	0.0487 (15)	0.0611 (17)	0.0465 (16)	-0.0117 (12)	0.0067 (12)	-0.0028 (13)
C13	0.157 (4)	0.062 (2)	0.086 (3)	0.016 (2)	0.057 (3)	0.002 (2)
C7	0.0661 (19)	0.073 (2)	0.0571 (19)	-0.0133 (15)	0.0270 (16)	-0.0028 (15)
C5	0.0522 (16)	0.080 (2)	0.0426 (16)	0.0032 (14)	0.0011 (13)	-0.0013 (14)
C14	0.080 (2)	0.068 (2)	0.065 (2)	0.0041 (16)	0.0277 (18)	0.0069 (16)
C12	0.193 (5)	0.053 (2)	0.063 (2)	-0.025 (3)	0.039 (3)	-0.0082 (17)
C11	0.120 (3)	0.074 (2)	0.062 (2)	-0.040 (2)	0.004 (2)	-0.0026 (18)
S1	0.0430 (4)	0.0810 (5)	0.0379 (4)	-0.0120 (3)	0.0064 (3)	0.0061 (3)
O2	0.0724 (14)	0.0939 (17)	0.0528 (13)	-0.0361 (12)	0.0013 (11)	0.0181 (11)
O1	0.0492 (11)	0.1182 (18)	0.0501 (12)	0.0083 (11)	0.0201 (10)	-0.0003 (12)
C15	0.0441 (14)	0.0618 (16)	0.0341 (13)	-0.0061 (12)	0.0040 (11)	0.0036 (12)
C19	0.0581 (18)	0.0678 (19)	0.062 (2)	0.0121 (14)	0.0142 (16)	0.0040 (15)
C20	0.0605 (18)	0.0576 (17)	0.0497 (17)	-0.0025 (13)	0.0077 (14)	-0.0031 (13)
C18	0.0455 (15)	0.079 (2)	0.0522 (18)	-0.0030 (15)	0.0040 (13)	0.0099 (16)
C16	0.0529 (16)	0.078 (2)	0.0465 (17)	0.0060 (14)	0.0023 (13)	-0.0129 (14)
C17	0.0566 (17)	0.085 (2)	0.0548 (19)	-0.0065 (16)	-0.0054 (14)	-0.0188 (16)
C21	0.0491 (18)	0.127 (3)	0.088 (3)	0.000 (2)	-0.0033 (18)	0.009 (2)
Br	0.0854 (3)	0.0743 (2)	0.0511 (2)	-0.02668 (16)	0.01018 (17)	-0.01482 (14)

Geometric parameters (\AA , $^\circ$)

C1—C2	1.330 (4)	C5—H5	0.93
C1—C9	1.483 (4)	C14—H14	0.93

C1—S1	1.793 (3)	C12—C11	1.362 (6)
C9—C10	1.379 (4)	C12—H12	0.93
C9—C14	1.382 (4)	C11—H11	0.93
C3—C8	1.381 (3)	S1—O1	1.426 (2)
C3—C4	1.386 (3)	S1—O2	1.430 (2)
C3—C2	1.483 (3)	S1—C15	1.762 (3)
C2—Br	1.901 (3)	C15—C16	1.365 (4)
C4—C5	1.374 (4)	C15—C20	1.382 (4)
C4—H4	0.93	C19—C20	1.365 (4)
C6—C5	1.361 (4)	C19—C18	1.373 (4)
C6—C7	1.381 (4)	C19—H19	0.93
C6—H6	0.93	C20—H20	0.93
C10—C11	1.380 (5)	C18—C17	1.368 (4)
C10—H10	0.93	C18—C21	1.512 (4)
C8—C7	1.373 (4)	C16—C17	1.382 (4)
C8—H8	0.93	C16—H16	0.93
C13—C12	1.356 (6)	C17—H17	0.93
C13—C14	1.367 (5)	C21—H21A	0.96
C13—H13	0.93	C21—H21B	0.96
C7—H7	0.93	C21—H21C	0.96
C2—C1—C9	121.2 (2)	C13—C12—C11	120.2 (4)
C2—C1—S1	124.1 (2)	C13—C12—H12	119.9
C9—C1—S1	114.63 (18)	C11—C12—H12	119.9
C10—C9—C14	118.7 (3)	C12—C11—C10	119.8 (4)
C10—C9—C1	120.9 (3)	C12—C11—H11	120.1
C14—C9—C1	120.3 (3)	C10—C11—H11	120.1
C8—C3—C4	119.2 (2)	O1—S1—O2	118.75 (14)
C8—C3—C2	120.9 (2)	O1—S1—C15	108.95 (13)
C4—C3—C2	119.9 (2)	O2—S1—C15	107.45 (14)
C1—C2—C3	124.9 (2)	O1—S1—C1	109.93 (13)
C1—C2—Br	122.9 (2)	O2—S1—C1	105.77 (12)
C3—C2—Br	112.19 (18)	C15—S1—C1	105.13 (11)
C5—C4—C3	120.0 (2)	C16—C15—C20	120.4 (2)
C5—C4—H4	120.0	C16—C15—S1	120.1 (2)
C3—C4—H4	120.0	C20—C15—S1	119.5 (2)
C5—C6—C7	119.4 (3)	C20—C19—C18	121.8 (3)
C5—C6—H6	120.3	C20—C19—H19	119.1
C7—C6—H6	120.3	C18—C19—H19	119.1
C9—C10—C11	120.3 (3)	C19—C20—C15	119.1 (3)
C9—C10—H10	119.8	C19—C20—H20	120.5
C11—C10—H10	119.8	C15—C20—H20	120.5
C7—C8—C3	120.1 (3)	C17—C18—C19	118.0 (3)
C7—C8—H8	120.0	C17—C18—C21	121.5 (3)
C3—C8—H8	120.0	C19—C18—C21	120.5 (3)
C12—C13—C14	120.7 (4)	C15—C16—C17	119.1 (3)
C12—C13—H13	119.6	C15—C16—H16	120.4
C14—C13—H13	119.6	C17—C16—H16	120.4
C8—C7—C6	120.5 (3)	C18—C17—C16	121.5 (3)
C8—C7—H7	119.8	C18—C17—H17	119.2

supplementary materials

C6—C7—H7	119.8	C16—C17—H17	119.2
C6—C5—C4	120.9 (3)	C18—C21—H21A	109.5
C6—C5—H5	119.5	C18—C21—H21B	109.5
C4—C5—H5	119.5	H21A—C21—H21B	109.5
C13—C14—C9	120.1 (4)	C18—C21—H21C	109.5
C13—C14—H14	119.9	H21A—C21—H21C	109.5
C9—C14—H14	119.9	H21B—C21—H21C	109.5
C2—C1—C9—C10	-105.1 (3)	C14—C13—C12—C11	1.3 (6)
S1—C1—C9—C10	77.0 (3)	C13—C12—C11—C10	-1.4 (6)
C2—C1—C9—C14	75.1 (3)	C9—C10—C11—C12	1.1 (5)
S1—C1—C9—C14	-102.8 (3)	C2—C1—S1—O1	45.3 (2)
C9—C1—C2—C3	3.9 (4)	C9—C1—S1—O1	-136.93 (19)
S1—C1—C2—C3	-178.41 (19)	C2—C1—S1—O2	174.6 (2)
C9—C1—C2—Br	-176.77 (18)	C9—C1—S1—O2	-7.6 (2)
S1—C1—C2—Br	0.9 (3)	C2—C1—S1—C15	-71.9 (2)
C8—C3—C2—C1	-122.7 (3)	C9—C1—S1—C15	105.9 (2)
C4—C3—C2—C1	58.0 (4)	O1—S1—C15—C16	-3.0 (3)
C8—C3—C2—Br	57.9 (3)	O2—S1—C15—C16	-132.9 (2)
C4—C3—C2—Br	-121.4 (2)	C1—S1—C15—C16	114.8 (2)
C8—C3—C4—C5	0.2 (4)	O1—S1—C15—C20	175.4 (2)
C2—C3—C4—C5	179.5 (3)	O2—S1—C15—C20	45.5 (2)
C14—C9—C10—C11	-0.7 (5)	C1—S1—C15—C20	-66.8 (2)
C1—C9—C10—C11	179.5 (3)	C18—C19—C20—C15	1.6 (5)
C4—C3—C8—C7	-0.1 (4)	C16—C15—C20—C19	-0.9 (4)
C2—C3—C8—C7	-179.4 (3)	S1—C15—C20—C19	-179.2 (2)
C3—C8—C7—C6	0.1 (5)	C20—C19—C18—C17	-1.1 (5)
C5—C6—C7—C8	-0.3 (5)	C20—C19—C18—C21	179.5 (3)
C7—C6—C5—C4	0.4 (5)	C20—C15—C16—C17	-0.4 (4)
C3—C4—C5—C6	-0.4 (4)	S1—C15—C16—C17	178.0 (2)
C12—C13—C14—C9	-0.9 (6)	C19—C18—C17—C16	-0.2 (5)
C10—C9—C14—C13	0.6 (5)	C21—C18—C17—C16	179.2 (3)
C1—C9—C14—C13	-179.6 (3)	C15—C16—C17—C18	0.9 (5)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12 \cdots Cg1 ⁱ	0.93	2.91	3.608 (5)	133
C19—H19 \cdots Cg1 ⁱⁱ	0.93	2.88	3.786 (4)	166

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

Fig. 1

