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N-(2-Bromophenyl)-4-methyl-*N*-(4-methylphenylsulfonyl)benzenesulfonamide

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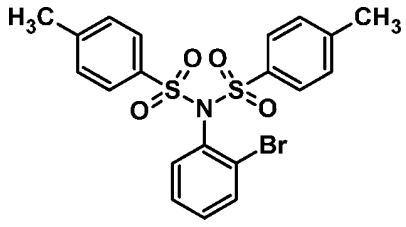
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.038; wR factor = 0.085; data-to-parameter ratio = 15.9.

In the title compound, $C_{20}H_{18}BrNO_4S_2$, the mean planes formed by the toluene substituents are inclined at a dihedral angle of 45.34 (8)°. The bromobenzene group is disordered over two positions with an occupancy ratio of 0.74:0.26, resulting in two conformations of the ring; the two rings are oriented at a dihedral angle of 6.6 (6)° with each other. In the crystal structure, weak C—H···O interactions connect the molecules in a zigzag manner along the *a* axis.

Related literature

For general background, see: Ames & Opalko (1984); Arshad *et al.* (2011). For related structures, see: Zhao *et al.* (2007); Song (2008); Hanson & Hitchcock (2004).



Experimental

Crystal data

$C_{20}H_{18}BrNO_4S_2$
M_r = 480.38
Monoclinic, $P2_1/c$
a = 10.5819 (15) Å
b = 13.1465 (19) Å
c = 14.235 (2) Å
β = 95.478 (2)°
V = 1971.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.32 mm^{-1}
T = 100 K
0.38 × 0.33 × 0.24 mm

Data collection

Bruker KAPPA APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.472, T_{max} = 0.605
23193 measured reflections
4792 independent reflections
4320 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.085
S = 1.24
4792 reflections
301 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3^{i}	0.95	2.45	3.199 (3)	135

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

Data collection: *APEX2* (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: *PLATON* (Spek, 2009) and *X-SEED* (Barbour, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2443).

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