organic compounds

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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, C20H18BrNO4S2, 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

C20H18BrNO4S2
V = 1971.2 (5) Å³
M_r = 480.38
Monoclinic, P2_1/c
Mo Kα radiation
a = 10.5819 (15) Å
μ = 2.32 mm⁻¹
b = 13.1465 (19) Å
T = 100 K
c = 14.235 (2) Å
0.38 × 0.33 × 0.24 mm
β = 95.478 (2)°

Data collection

Bruker KAPPA APEXII CCD diffractometer
4792 independent reflections
Absorption correction: multi-scan
4792 reflections with I > 2σ(I)
(SADABS; Bruker, 2001)
Tmin = 0.472, Tmax = 0.605

Refinement

R[F² > 2σ(F²)] = 0.038
wR(F²) = 0.085
S = 1.24
301 parameters
4792 reflections
H-atom parameters constrained
Δρ_max = 0.52 e Å⁻³
Δρ_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⋯O3i
0.95
2.45
3.199 (3)
135

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

References