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3-(2,4-Dichlorophenyl)-*N*,*N*-diethyl-3-(4-methylphenylsulfonylamino)propanamide

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The S atom of the sulfonyl group in the title compound, $C_{20}H_{24}Cl_2N_2O_3S$, has a distorted tetrahedral geometry. Two intermolecular N—H···O hydrogen bonds between the amino groups and the carbonyl groups link the molecules into a centrosymmetric dimer.

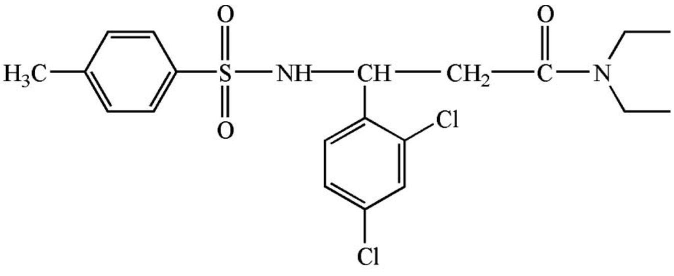
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.132
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The addition of a nucleophile to unsaturated carbon–nitrogen bonds is a convenient method of synthesizing amine derivatives (Kobayashi & Ishitani, 1999). In our laboratory, we have recently investigated a new metal-mediated reaction for the preparation of β-sulfonylaminoamides. The title compound, (I), has been synthesized by the reaction of *N*-(2,4-dichlorobenzylidene)-4-methylbenzenesulfonamide and 2-bromo-*N*,*N*-diethylacetamide in the presence of zinc powder.



(I)

The molecular structure of (I) and the atom-numbering scheme are shown in Fig. 1. In this structure, the benzene ring attached to the sulfonyl group makes a dihedral angle of 11.7 (3)° with the dichlorophenyl ring. The S atom has a distorted tetrahedral geometry, with the O2—S1—O1 and O2—S1—N1 angles (Table 1) deviating most from the regular tetrahedral value. Intermolecular N—H···O hydrogen bonds are formed between the amino groups and the carbonyl groups of two molecules, forming a centrosymmetric dimer.

Experimental

The title compound was synthesized by adding 2-bromo-*N*,*N*-diethylacetamide (3.0 mmol) to a solution of *N*-(2,4-dichlorobenzylidene)-4-methylbenzenesulfonamide (1.0 mmol) in dichloromethane (5.0 ml). Zinc powder (6.0 mmol) and a trace amount of iodine were added to the mixture. After the mixture had been refluxed for 6 h, the reaction was quenched with a saturated solution of ammonium chloride (8.0 ml). The mixture was extracted with dichloromethane, evaporated and separated by flash chromatography (using ethyl acetate–petroleum ether). A white powder (yield 64%) was obtained. Slow evaporation of a dichloromethane–petroleum ether (1:7) solution afforded the title compound as single crystals.

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Crystal data

$C_{20}H_{24}Cl_2N_2O_3S$
$M_r = 443.38$
Triclinic, $P\overline{1}$
$a = 7.895$ (3) Å
$b = 10.704$ (4) Å
$c = 14.046$ (4) Å
$\alpha = 105.881$ (5)°
$\beta = 100.025$ (4)°
$\gamma = 99.190$ (4)°
$V = 1097.0$ (7) Å^3
$Z = 2$
$D_x = 1.342$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.41$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.36 × 0.22 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.896$, $T_{max} = 0.944$
5569 measured reflections
3833 independent reflections
3131 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.132$
$S = 1.06$
3833 reflections
258 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.8034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.71$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.426 (2)	S1—N1	1.606 (2)
S1—O1	1.427 (2)	S1—C8	1.766 (3)
O2—S1—O1	120.48 (15)	O2—S1—C8	107.45 (13)
O2—S1—N1	105.55 (14)	O1—S1—C8	107.80 (14)
O1—S1—N1	107.42 (13)	N1—S1—C8	107.55 (12)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.79 (3)	2.04 (3)	2.806 (3)	166 (3)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

All carbon-bound H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.98 Å), with U_{iso}(H) set at $1.2U_{eq}$(C) or $1.5U_{eq}$(methyl C). The coordinates of atom H1 were refined. Methyl groups C14 and C18 were allowed to rotate but not to tip.

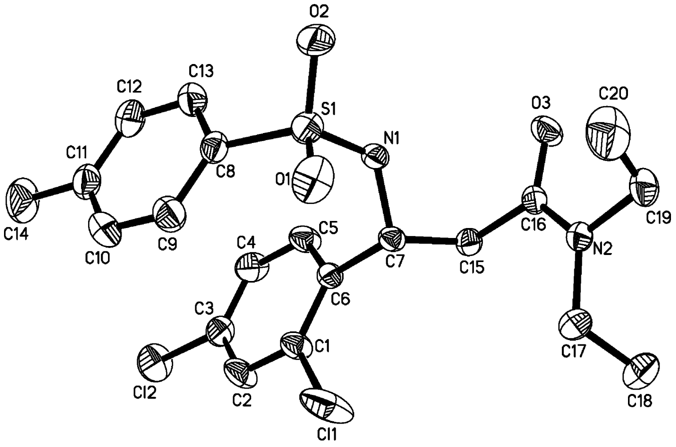

Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.

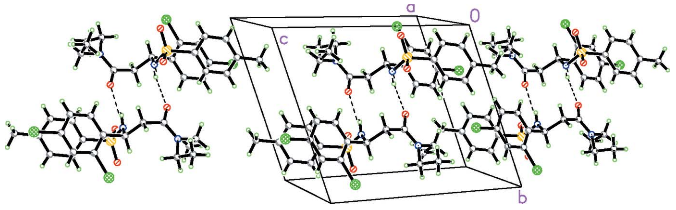

Figure 2
View of the molecular structure of (I). Dashed lines indicate N—H···O interactions.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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