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# A novel sulfonamide containing a boronate ester group

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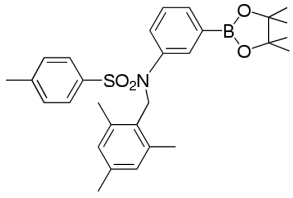
A novel sulfonamide containing a boronate ester group, namely *N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-phenyl]-*N*-(2,4,6-trimethylbenzyl)-*p*-toluenesulfonamide, $C_{29}H_{36}BNO_4S$, crystallizes with two independent molecules in the asymmetric unit. The Lewis-acid B atom is in a trigonal–planar environment and is not involved in inter- or secondary intramolecular interactions.




(I)

## Experimental

The title compound was prepared by the addition of *N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-*N*-(2,4,6-trimethylbenzyl)amine (400 mg, 1.14 mmol) to a stirred solution of *p*-toluenesulfonyl chloride (326 mg, 1.71 mmol) in 5 ml of $CH_2Cl_2$ at 273 K. Triethylamine (0.5 ml) was added and the solution was stirred overnight. The solvent was removed under vacuum and the title compound was crystallized from ether (5 ml) at 278 K. Yield: 66 mg (11%).

*Crystal data*

$C_{29}H_{36}BNO_4S$
$M_r$ = 505.46
Triclinic, $P\overline{1}$
$a$ = 12.7798 (9) Å
$b$ = 14.4877 (10) Å
$c$ = 16.5149 (12) Å
$\alpha$ = 66.858 (2)°
$\beta$ = 86.916 (2)°
$\gamma$ = 85.396 (2)°
$V$ = 2801.8 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.198 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 9524 reflections
$\theta$ = 2.3–33.2°
$\mu$ = 0.15 mm$^{-1}$
$T$ = 173 (2) K
Block, colourless
0.45 × 0.40 × 0.35 mm

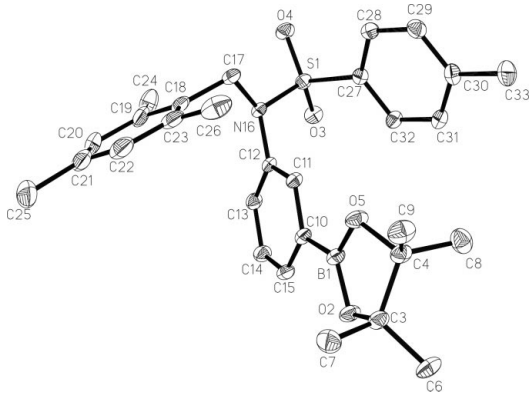



**Figure 1**
A view of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted.

**Key indicators**

Single-crystal X-ray study
$T$ = 173 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.053
$wR$ factor = 0.154
Data-to-parameter ratio = 29.1

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

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 11889 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.022$ |
| Absorption correction: none | $\theta_{max} = 32.5^\circ$ |
| 30001 measured reflections | $h = -19 \rightarrow 18$ |
| 19380 independent reflections | $k = -21 \rightarrow 21$ |
| | $l = -23 \rightarrow 24$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.053$ | $w = 1/[\sigma^2(F_o^2) + (0.0893P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.154$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $S = 0.95$ | $\Delta\rho_{max} = 0.70$ e Å$^{-3}$ |
| 19380 reflections | $\Delta\rho_{min} = -0.47$ e Å$^{-3}$ |
| 665 parameters | |

Data collection: *SMART* (Bruker, 1997–1999); cell refinement: *SMART*; data reduction: *SHELXTL* (Sheldrick, 1997*a*); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*b*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

## References

Bruker (1997–1999). *SMART*. Version 5.059. Bruker AXS Inc., Madison, Wisconsin, USA.

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